Towards Flexible Interfacing of Machine Learning with Land Models

David Lawrence
CESM Chief Scientist

LSMS 2022
LAND SURFACE MODELLING SUMMIT

September, 2022

Eleanor Blyth and David Lawrence

***Steering Committee:* Aaron Boone, Simon Dadson, Rosie Fisher, Martin de Kauwe, Julia Pongratz, Kei Yoshimura**

***Administrative Support:* Victoria Barlow, Marcia Spencer**

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Land and Earth System models are increasingly being asked to provide information on societally-relevant impacts and adaptation associated with climate and environmental change

- Ecosystem vulnerability and impacts on carbon cycle and ecosystem services
- Water and food security in context of climate variability, change, and extreme weather
- Land-based mitigation solutions (net-zero targets); Impacts of land use and land-use change on climate, carbon, water, and extremes
- Hazard prediction (drought, floods, fire, heat waves, etc) under a changing climate
- *Understand and exploit sources of predictability from land processes, Earth System prediction*

nature

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EDITORIAL | 16 August 2022

We must get a grip on forest science – before it's too late

Trees are one of our biggest carbon hopes. Supporting the scientists studying them should be a much higher priority.

Will we have enough water?

Will we be able to produce enough food?

Where and when will people and ecoystems experience more extreme events?

Where are we going to put the carbon (and will it stay there)?

JAMES | Journal of Advances in Modeling Earth Systems

Commissioned Manuscript | Open Access

Perspectives on the Future of Land Surface Models and the Challenges of Representing Complex Terrestrial Systems

Rosie A. Fisher, Charles D. Koven

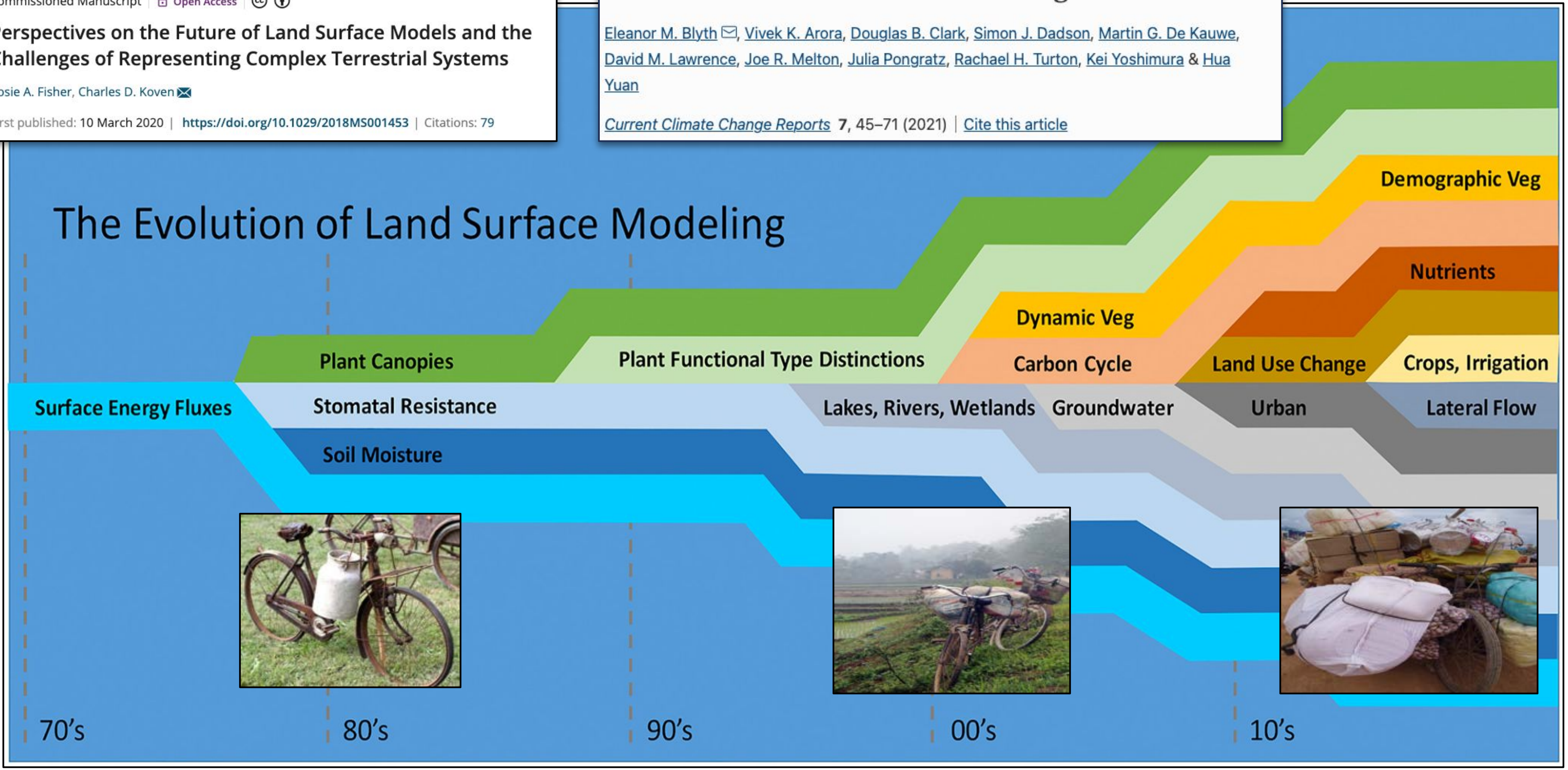
First published: 10 March 2020 | https://doi.org/10.1029/2018MS001453 | Citations: 79

Advances and Future Directions in Earth System Modelling (I Simpson, Section Editor) | Open Access | Published: 11 May 2021

Advances in Land Surface Modelling

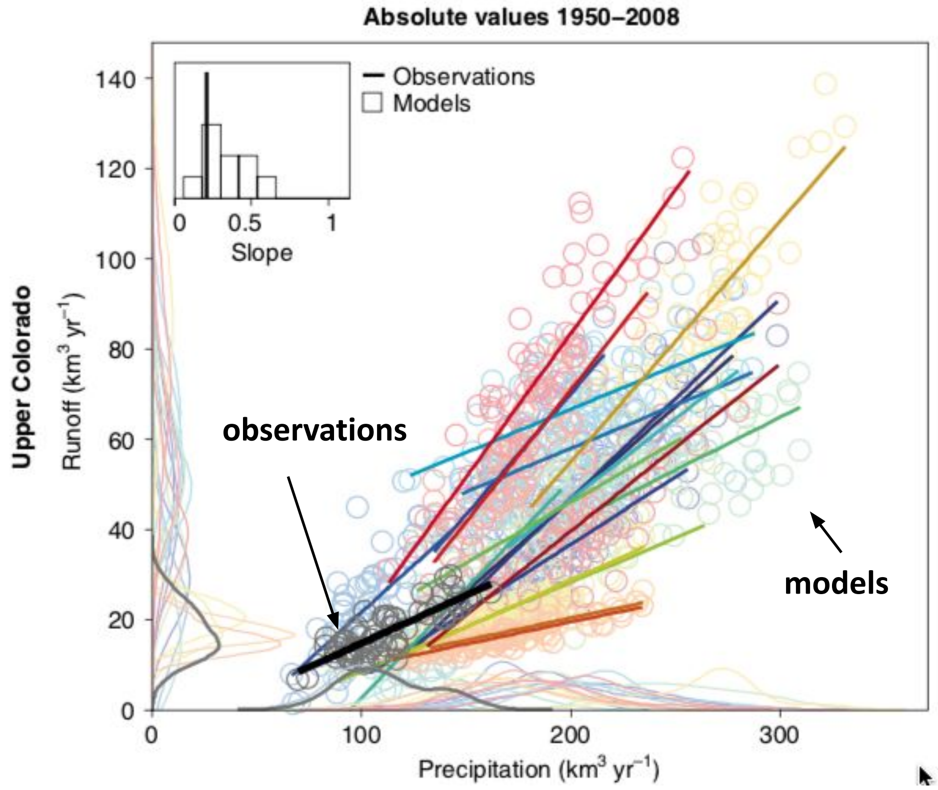
Eleanor M. Blyth, Vivek K. Arora, Douglas B. Clark, Simon J. Dadson, Martin G. De Kauwe, David M. Lawrence, Joe R. Melton, Julia Pongratz, Rachael H. Turton, Kei Yoshimura & Hua Yuan

Current Climate Change Reports 7, 45–71 (2021) | Cite this article



Will we have enough water?

Example actionable science limitation:
ESMs do not accurately simulate hydrologic sensitivity



CMIP models do not accurately represent changes in runoff associated with changes in P or T, which limits usability of runoff projections for adaptation purposes


PERSPECTIVE
https://doi.org/10.1038/s41558-019-0639-x
nature climate change

The potential to reduce uncertainty in regional runoff projections from climate models

Flavio Lehner[1,2,3]*, Andrew W. Wood[2], Julie A. Vano[2,4], David M. Lawrence[1], Martyn P. Clark[5] and Justin S. Mankin[6,7,8]

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Goal of the summit was to identify collaborative steps or activities that could be taken to **accelerate progress**

Focal Sessions

- New approaches for subgrid heterogeneity
- Managing model complexity
- Towards sharing of modules across LSMs
- Input and forcing datasets

- Crop modeling and forestry
- Water and land management
- Coupling external models to LSMs
- Fire and humans

- Land model benchmarking
- Machine learning approaches and LSMs
- Parameter estimation and uncertainty

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Recordings of presentations available from the conference webpage

https://hydro-jules.org/lsms2022-resources

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LAND SURFACE MODELLING SUMMIT

Goals of the Summit

Formal

- Collectively create a Road Map to address the challenges to improve land models so that they are fit for purpose to address scientific and societal needs associated with anthropogenically and naturally-driven environmental change
- Develop plans for follow up meetings and working groups, which can be used as basis for modeling groups and collaborative partners to solicit funding to support development activities and to build a community effort to accelerate progress

Informal

- Develop a shared understanding of the 'pain points' in modern land model development and application
- Foster collaborative relationships to address these challenges

Climate science is in transition

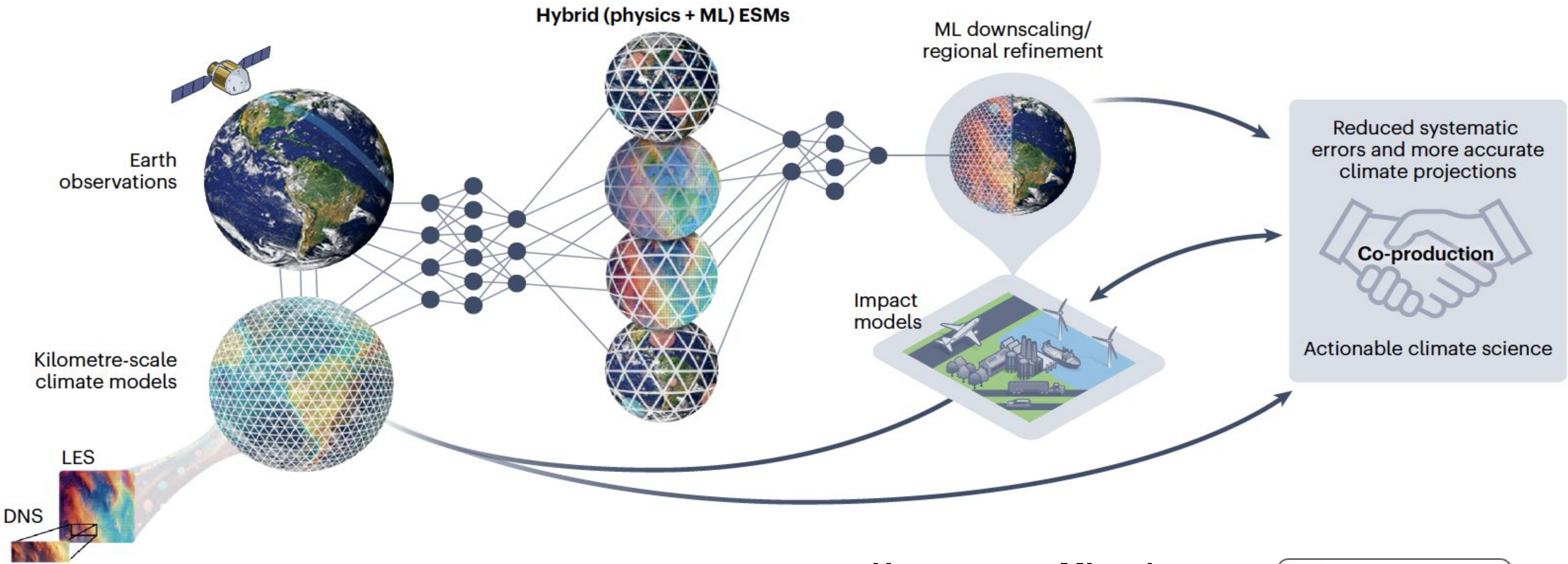
Urgent needs:

- actionable information (climate risks under different emissions scenarios; consequences of intervention/mitigation)
- more robust understanding of risks of tipping points

Yet, progress towards more accurate and reliable Earth System models remains slow

Image: Getty images

Next-generation Earth System modeling to address urgent mitigation and adaptation needs



Harness new ML + data to transform ESMs

Figure from Eyring, Gentine, Camps-Valls, Lawrence, Reichstein (Nature Climate Change, 2024)

*LEAP forward in the **reliability**, **utility**, and **reach** of climate projections through synergistic innovations in data science and climate science*

Next-generation Earth System modeling to address urgent mitigation and adaptation needs

So, what is needed to realize and accelerate the potential of ML to improve land modeling?

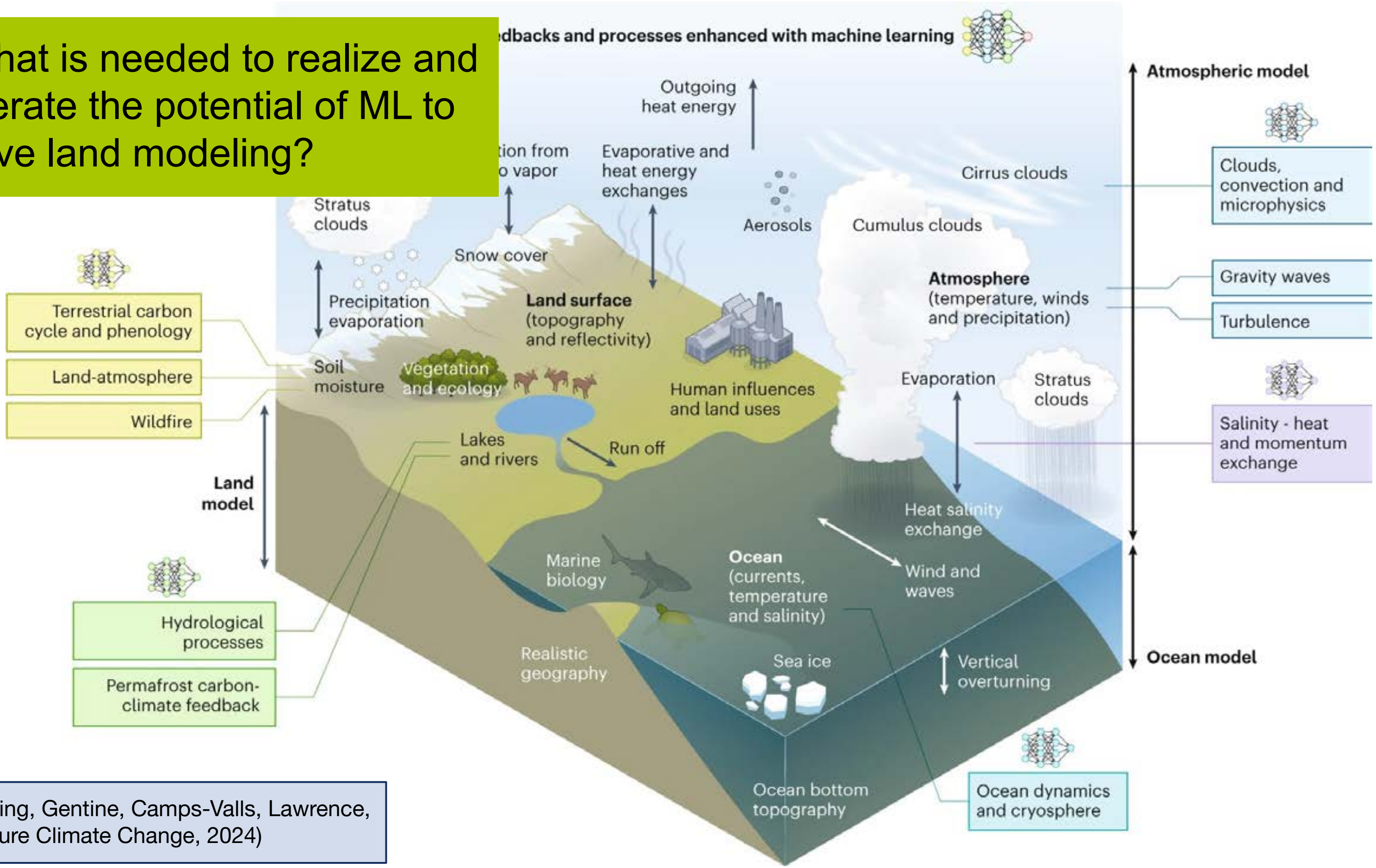


Figure from Eyring, Gentine, Camps-Valls, Lawrence, Reichstein (Nature Climate Change, 2024)

International Land Modelling Forum (ILMF)

The ILMF emerged from the Land Surface Modelling Summit in Oxford in Sept 2022. It provides a forum through which land modelling centres and researchers can interact and collaborate on mutually beneficial projects by

- **sharing ideas**
- **promoting relevant workshops and meetings**
- **advertising job opportunities**
- **coordinating working groups**

Initial working groups will focus on shareable modules, parameter estimation, the challenges of integrating humans into ESMs, and benchmarking.

LSMS 2022
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→
ILMF
INTERNATIONAL LAND MODELING FORUM

To join the ILMF, goto https://rebrand.ly/ILMF

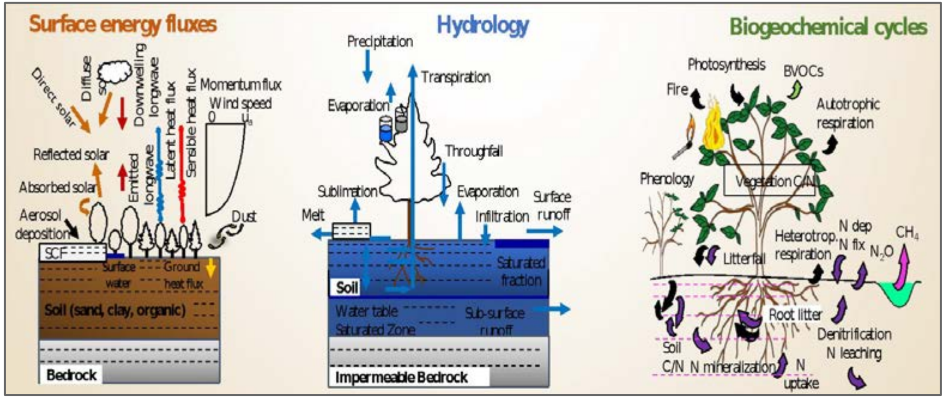
International Land Modelling Forum (ILMF) Interactive Webinars
September – October 2023

Available at https://hydro-jules.org/international-land-modeling-forum-ilmf

More accessible and modular code bases

So, what is needed to realize and accelerate the potential of ML to improve land modeling?

- Land model code bases are large, complex, and have legacies of 20+ years
  - 100's of thousands of lines of (Fortran!) code
  - Tangled code webs with lots of technical debt
- Code complexity and Fortran can be a barrier to entry for ML experts (or really anyone trying to advance the code)
  - Conversion to python-based language would be ideal, but costly
  - Cleaner and more modular code will help



Code Refactoring

Before

some_subroutine
calc. flux 1 … … … update state 1 calc. flux 2 … … … calc. flux 3 … … … update state 2

Slide credit Bill Sacks

Livable Code

https://brightonruby.com/2017/livable-code-sarah-mei/

You have to live here

Slide credit Bill Sacks

Livable Code

https://brightonruby.com/2017/livable-code-sarah-mei/

You **GET** to live here

Slide credit Bill Sacks

Pathways Towards Shareable Modules for Land Models

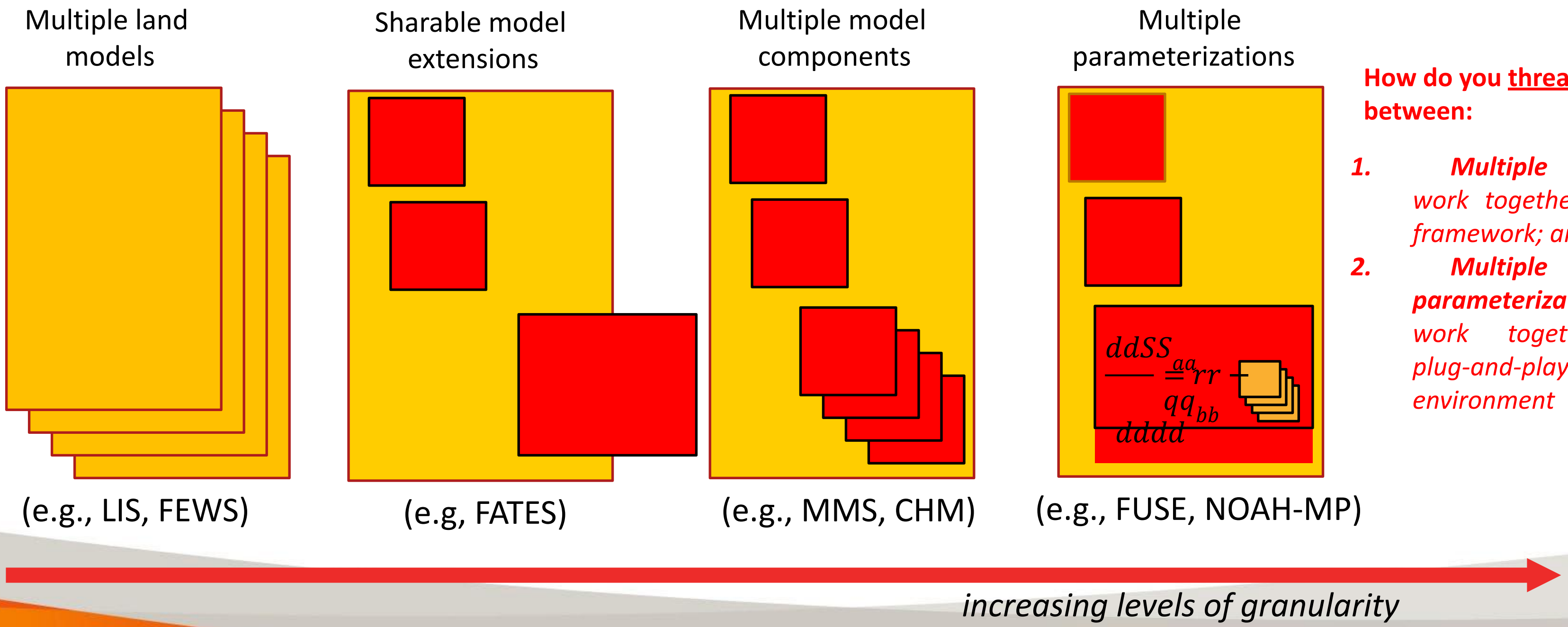
What do we mean by modularity?

Martyn P. Clark, PhD
Professor of Hydrology and Schulich Chair for Environmental Prediction
Department of Civil Engineering, Schulich School of Engineering, University of Calgary

21 September 2023

Unifying model physics

- **The problem**: A glut of hydrological models (Clark et al., WRR 2011) – in many cases there are more models in use than there are algorithms to populate them (same algorithms across multiple models)
- **The challenge:** Can we define a general "master modeling template" (general design principles) from which existing models can be constructed and new models derived (Clark et al., WRR 2015)?
- **The challenge:** Can we unify model building blocks across multiple levels of granularity?



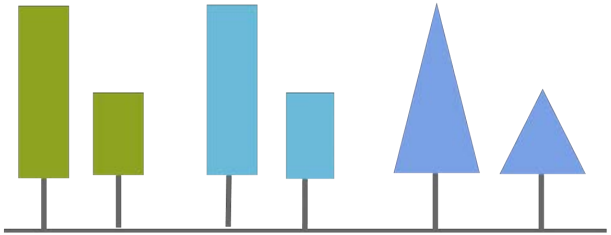
How do you <u>thread the needle</u> between:

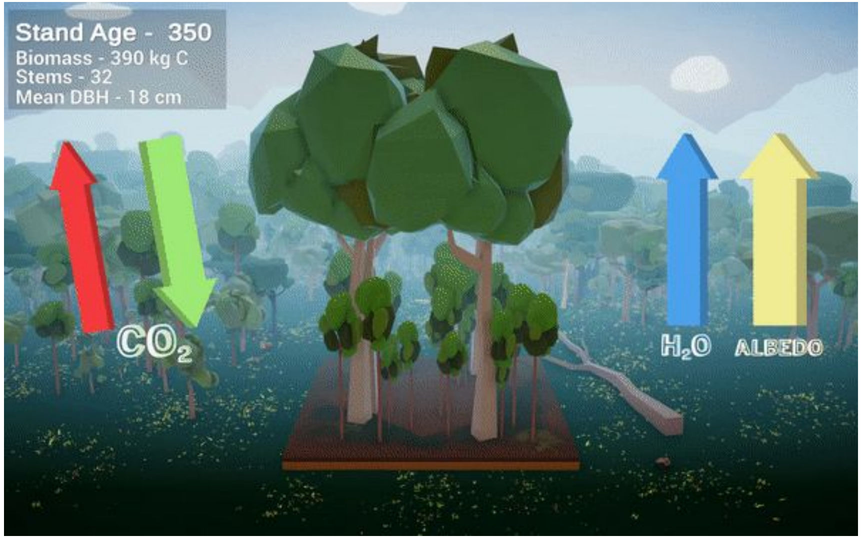
1. ***Multiple models*** *that work together in the same framework; and*
2. ***Multiple parameterizations*** *that work together in a plug-and-play environment*

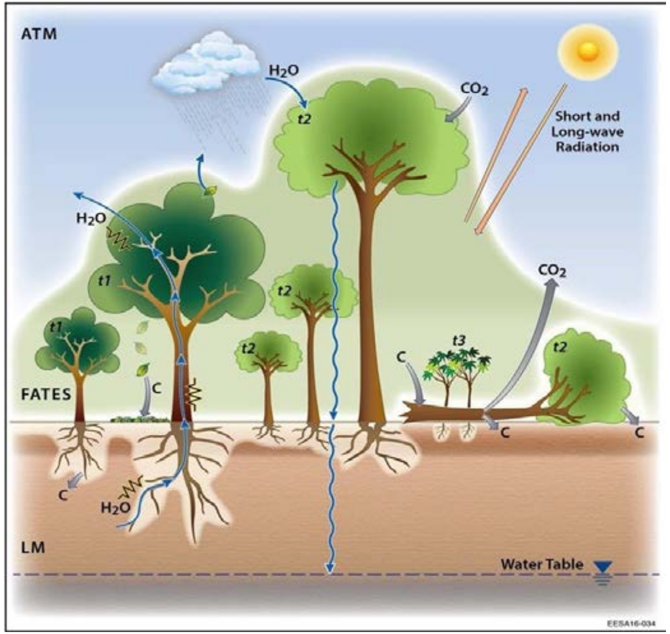
The Functionally Assembled Terrestrial Ecosystem Simulator (FATES): Modularity, Configurability, and Interoperability

C. Koven, R. Fisher, R. Knox,
B. Christoffersen, Y. Fang, A. Foster, J. Holm, E. Kluzek, L. Kueppers, D. Lawrence, G. Lemieux, S. Levis, M. Longo, J. Needham, W. Sacks, J. Shuman, M. Vertenstein, A. Walker, W. Wieder, C. Xu, and many others

FATES (Functionally Assembled Terrestrial Ecosystem Simulator)

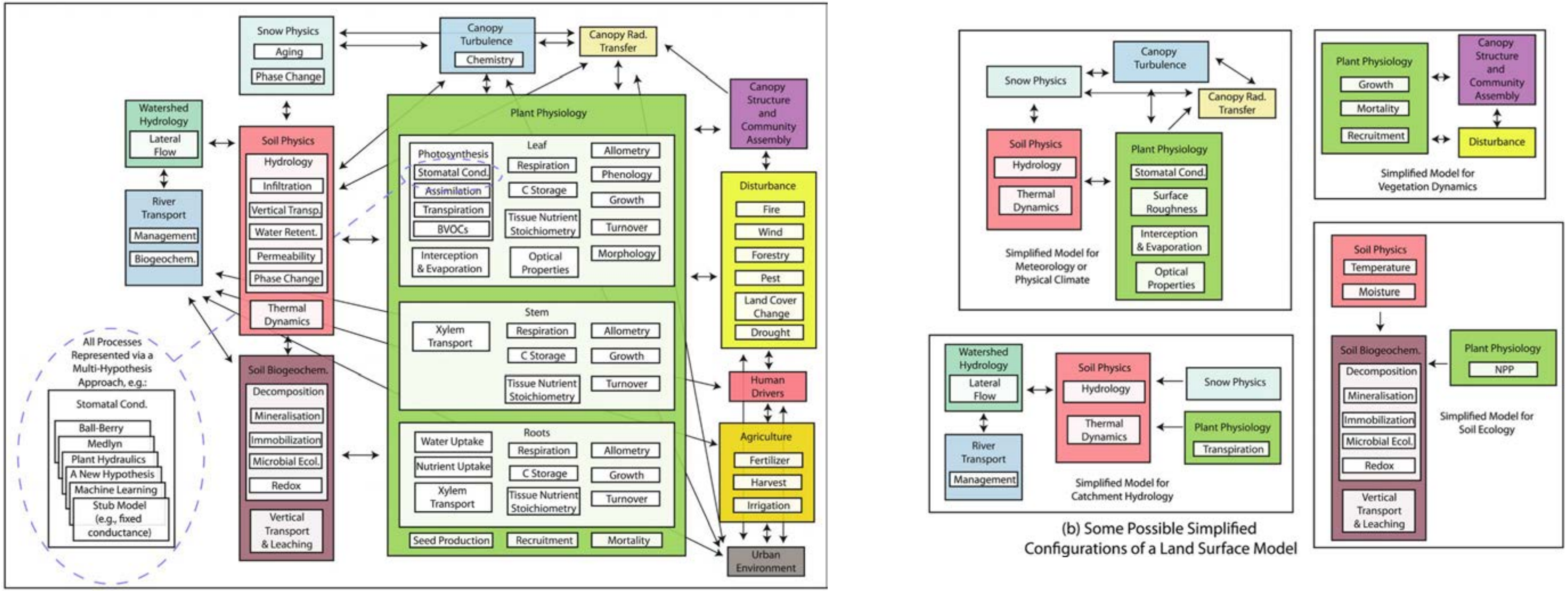






vegetation cohort-specific model (stand structure)
30-minute photosynthesis and fluxes
daily growth and allocation
competition and coexistence

Process-level modularity vs configurability
(We have focused on both with FATES)



Fisher and Koven, 2020

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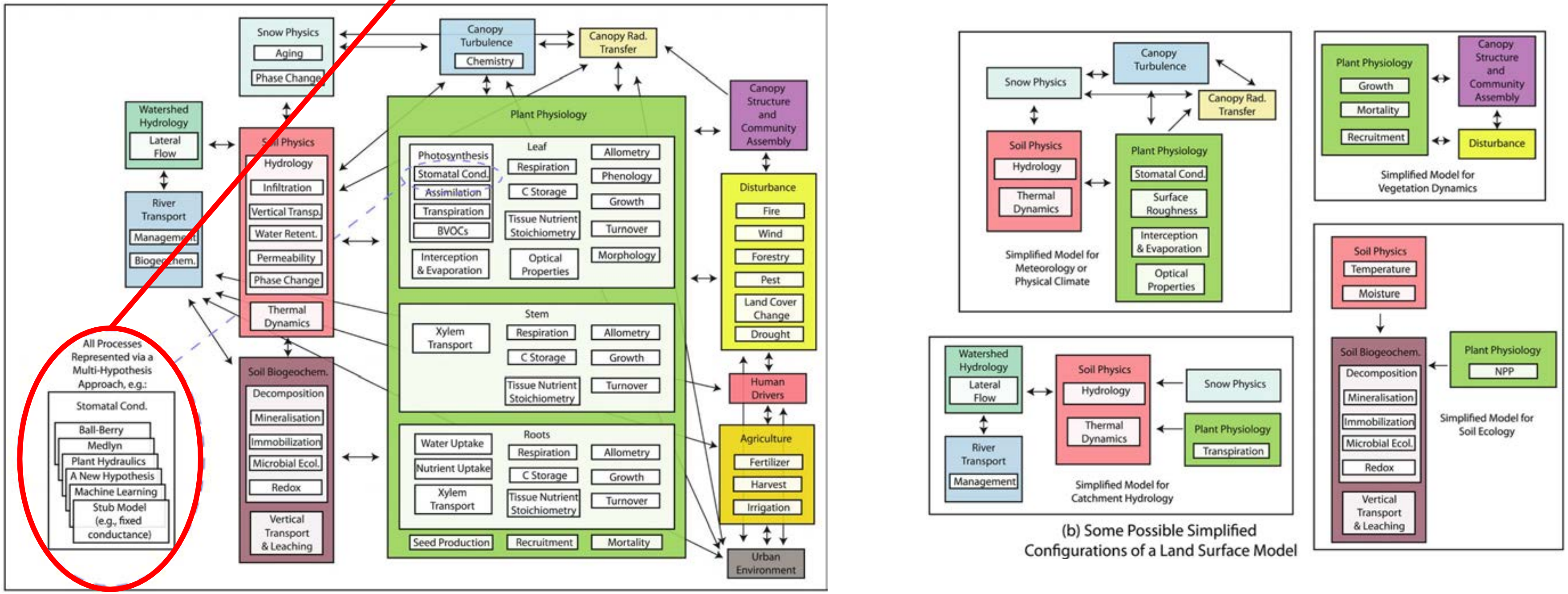
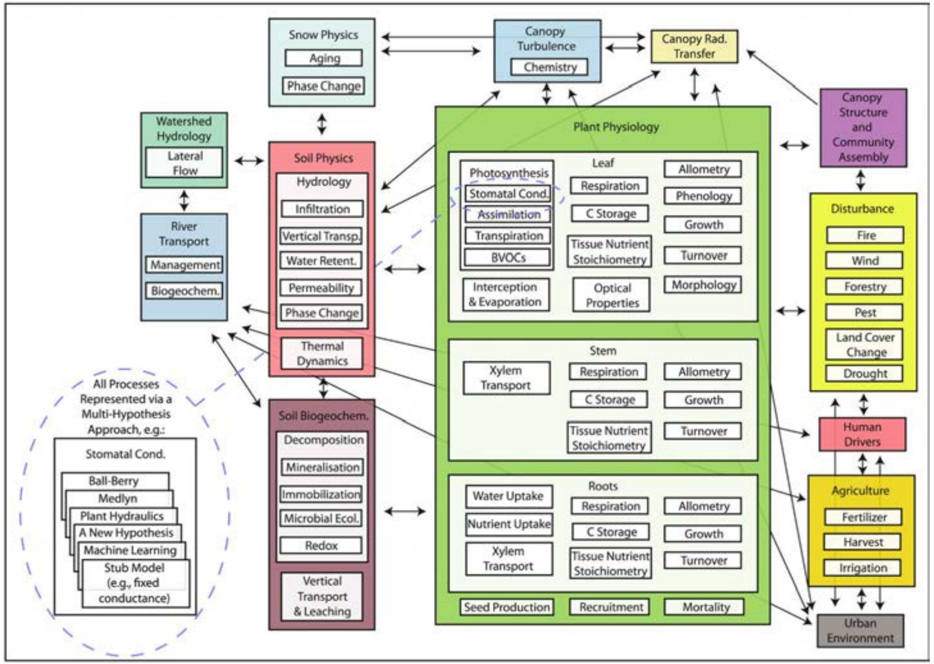
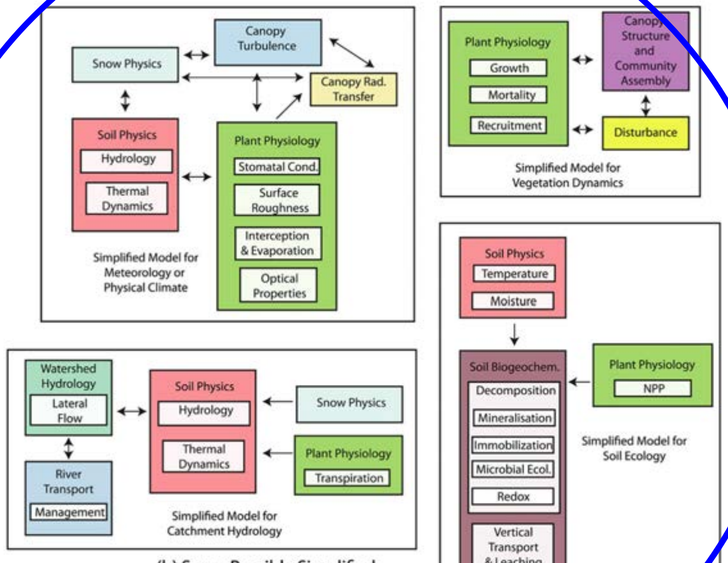


(b) Some Possible Simplified Configurations of a Land Surface Model

Fisher and Koven, 2020

Process-level modularity vs configurability
(We have focused on both with FATES)





(b) Some Possible Simplified Configurations of a Land Surface Model

Fisher and Koven, 2020

Modularisation in Land Surface models: discussion & future steps

Martyn Clark, Philippe Peylin, Dave Lawrence, Eleanor Blyth, Simon Dadson, Charlie Koven, Dai Yamazaki,...

Two possibles paths for international collaboration …

Global LSM

Individual processes

High level components
(ex. CamaFlood, FATES,...)

Intermediate level:
groups of processes
(ex. Snow dynamic, Leaf level photosynthesis, Soil C dyn., ...)

Low level:
Individual processes
(ex. process descriptions...)

Approach 1
"Top - down"

Define generic "Modules" with standard interfaces

Start with a concrete example (ex. Leaf phenology, SOM decomp.,..

Approach 2
"bottom up"

Building blocks towards a hybrid Earth System Model

Building blocks towards a hybrid Earth System Model

Robust and flexible Implementation of ML-based parameterizations requires Fortran-Python bridge

- FTorch implementation with CESM working fairly well
- To enable broad use, needs an integration plan to bring fully into CESM3 infrastructure
- Documentation for users
- Robust testing, edge-case evaluation
- GPU-CPU combo testing
- Ideally, some consistency in implementation of Fortran-Python bridge across modeling centers

The Community Land Model (CLM5) Parameter Perturbation Experiment

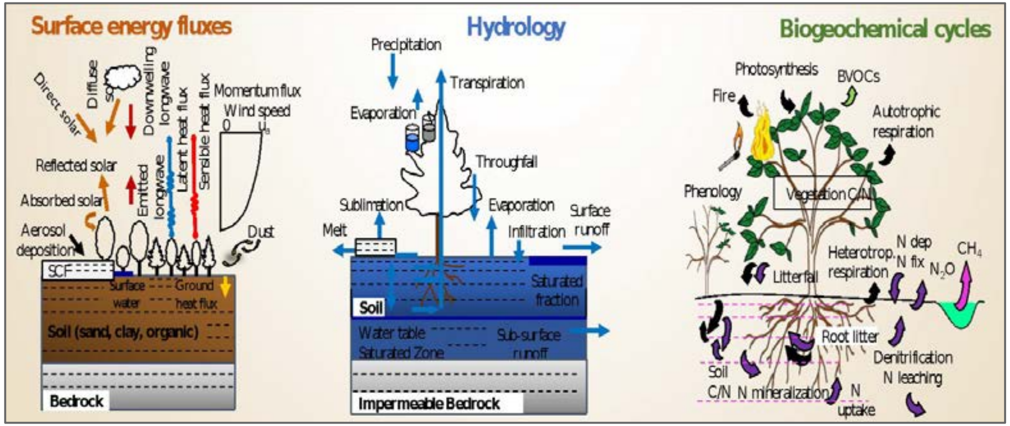
Quantifying parametric uncertainty and working towards automated calibration

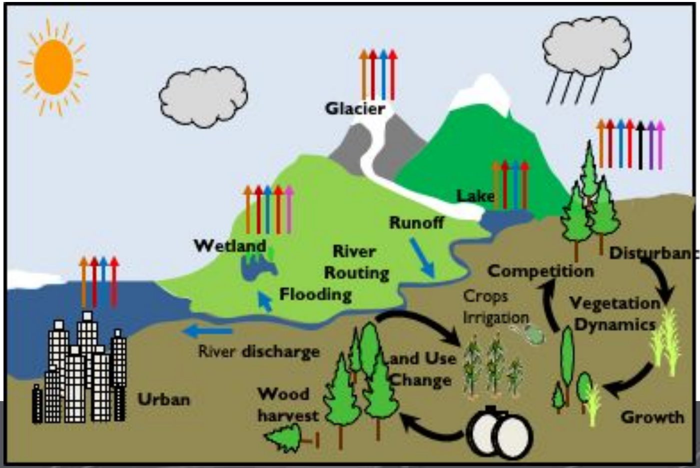
Linnia Hawkins, Daniel Kennedy, Katie Dagon

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 CLM PPE Project

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

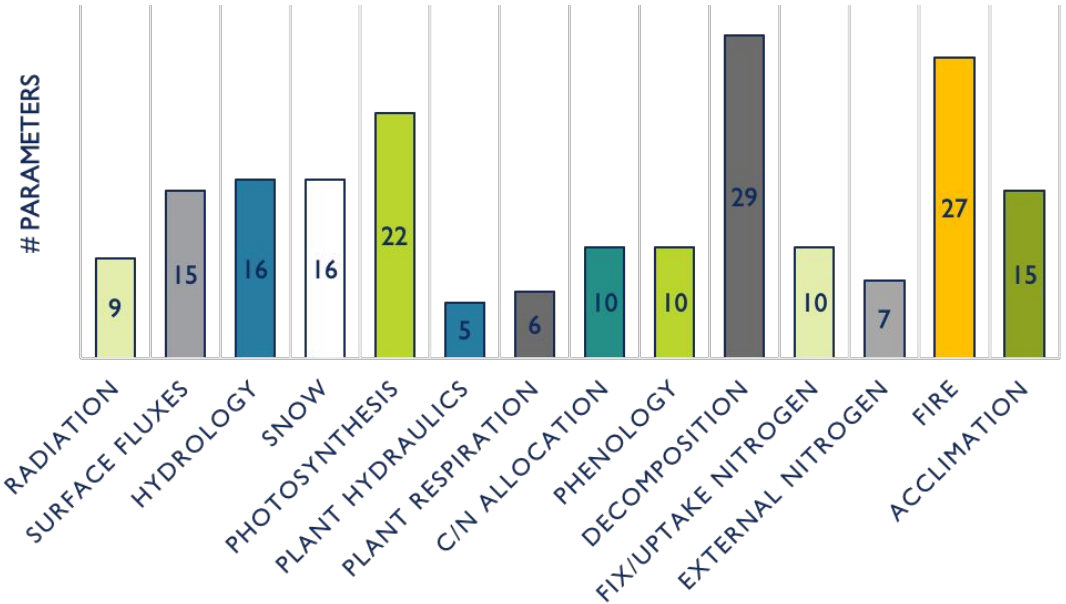




Motivation for the CLM PPE Project

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

CLM5(BGC) has over 200 parameters



Motivation for the CLM PPE Project

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

Drawbacks of hand tuning

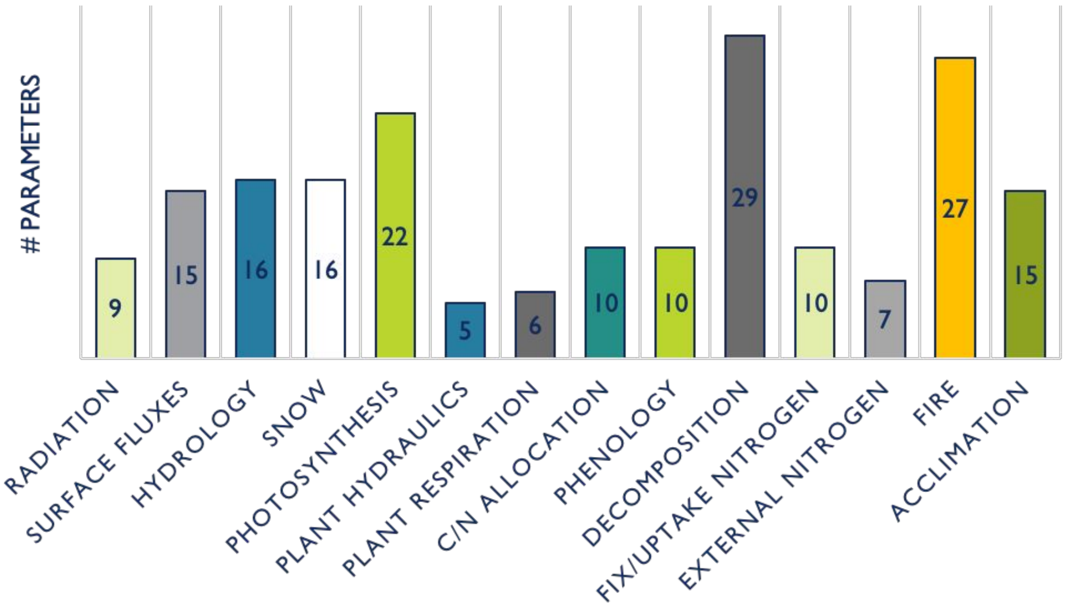
- Difficult to diagnose structural improvements

- Challenging to incorporate new parameterizations

- Impractical requisite knowledge base

- Doesn't scale well with increasing complexity

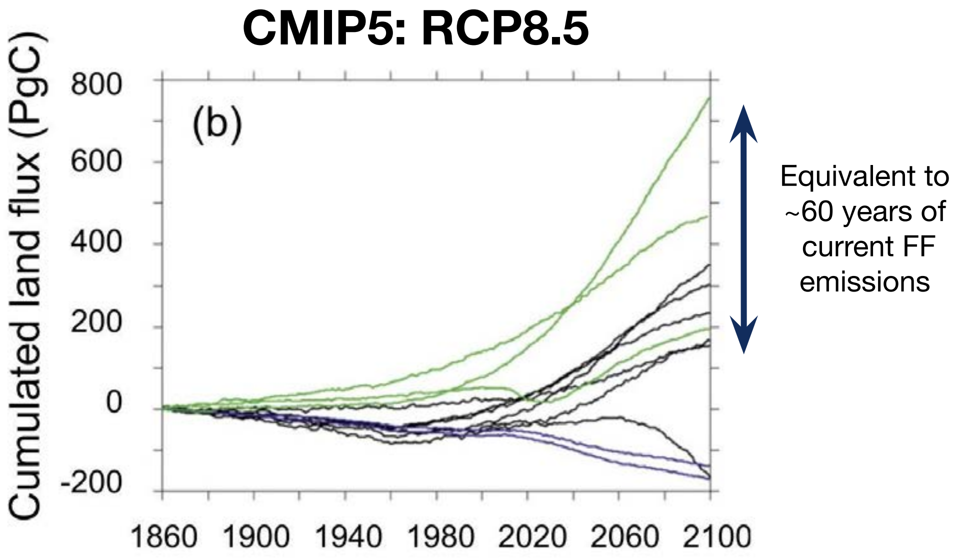
CLM5(BGC) has over 200 parameters



Motivation for the CLM PPE Project

- Growing complexity and comprehensiveness of land models → increasing # of uncertain 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 CLM PPE Project

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

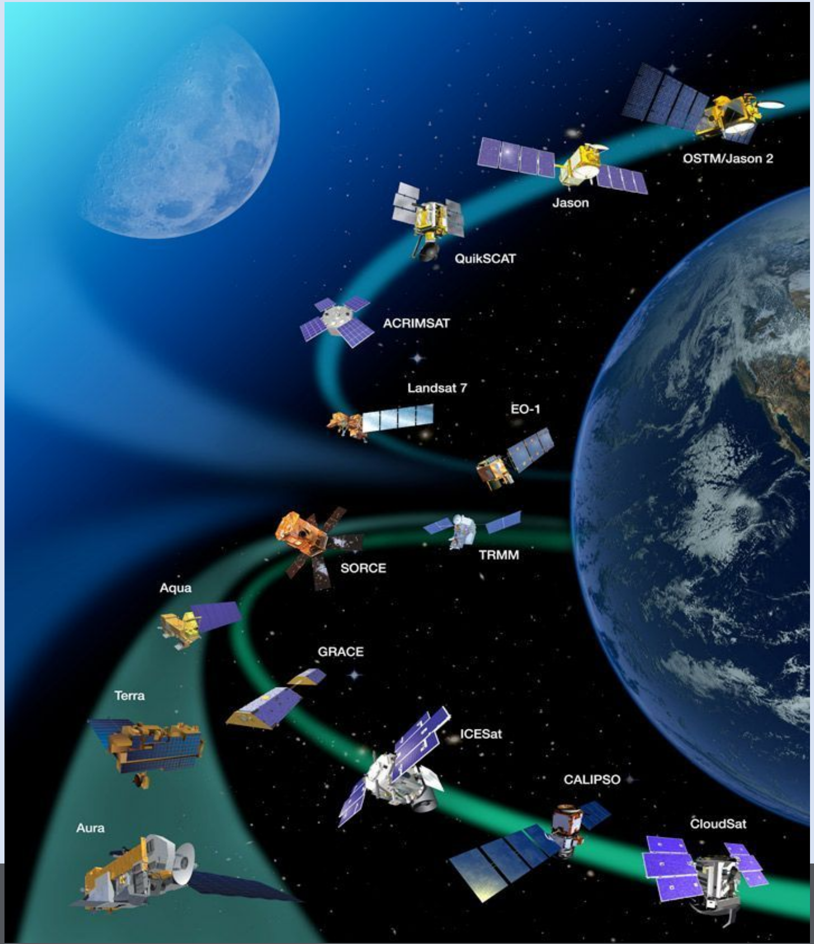
- Contribution of parameter uncertainty to total uncertainty expected to be large, but largely unquantified

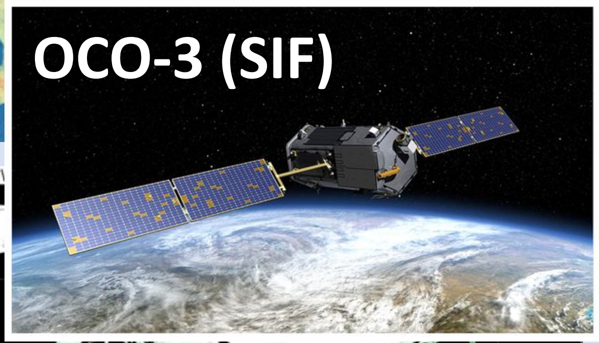
- Systematic parameter calibration will enhance accuracy of simulations, and increase suitability and accessibility of CLM for actionable science

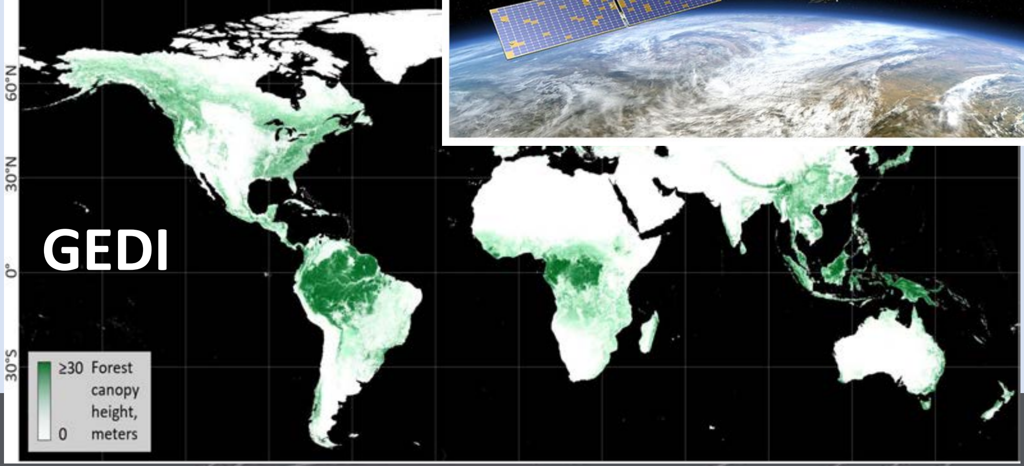
- Ecosystem vulnerability and impacts on carbon cycle and ecosystem services
- Water and food security in context of climate change, climate variability, and extreme weather
- Ecological, hydrological, and Earth system prediction
- Terrestrial contribution to Net Zero emissions goals

Unprecedented availability of Earth Observations

Unprecedented availability of Earth Observations

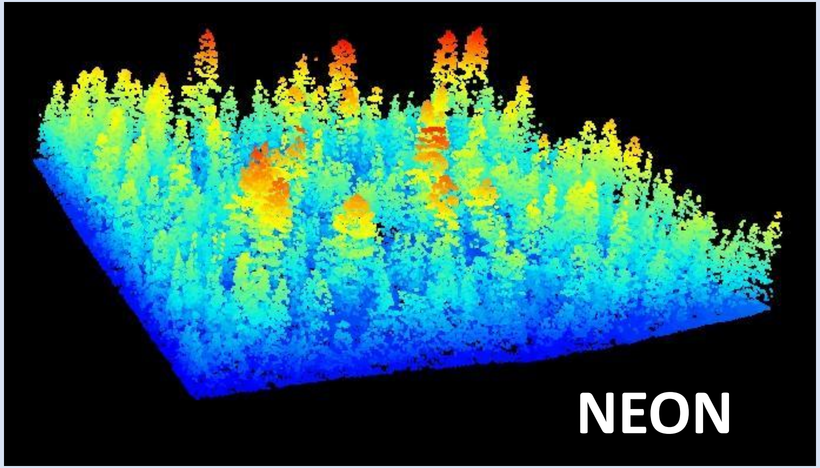




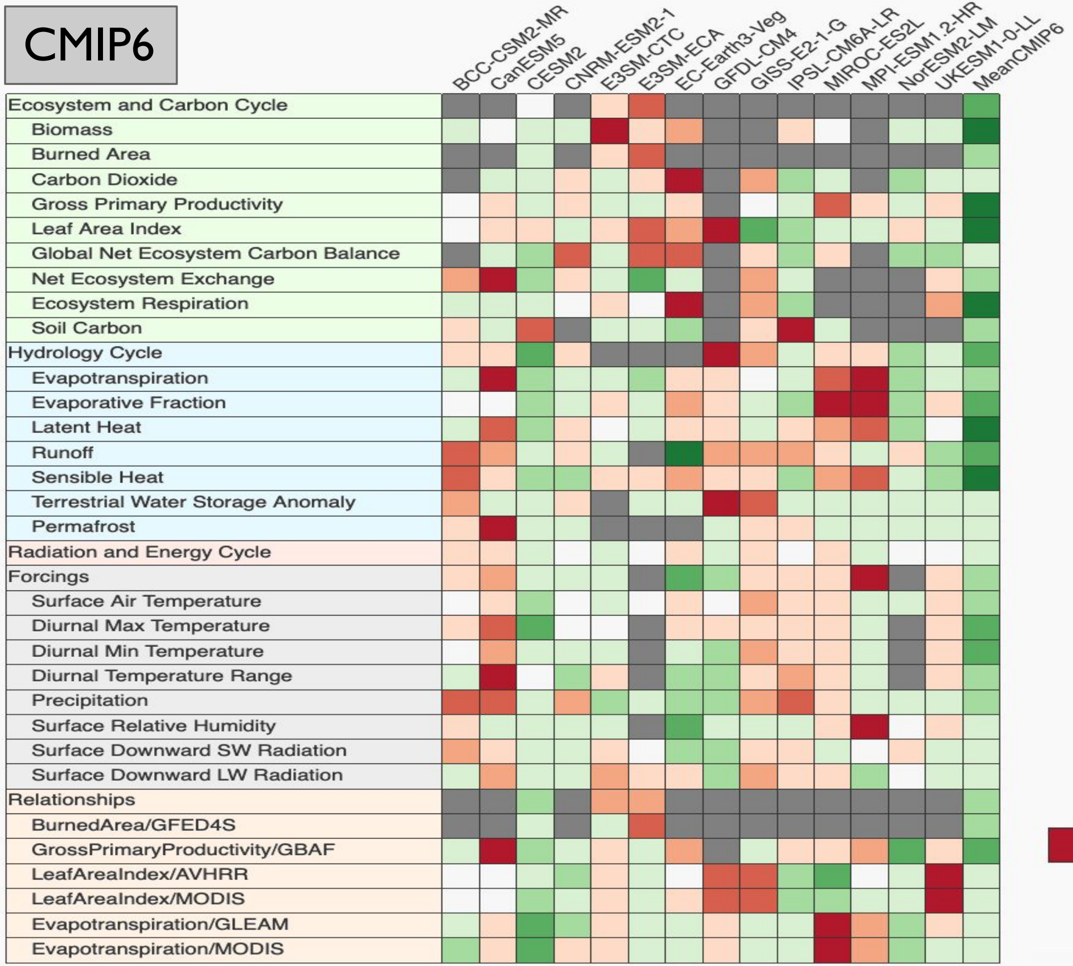


Unprecedented availability of Earth Observations

Flux tower networks like NEON, Ameriflux, FluxNet



And new integrated metrics packages



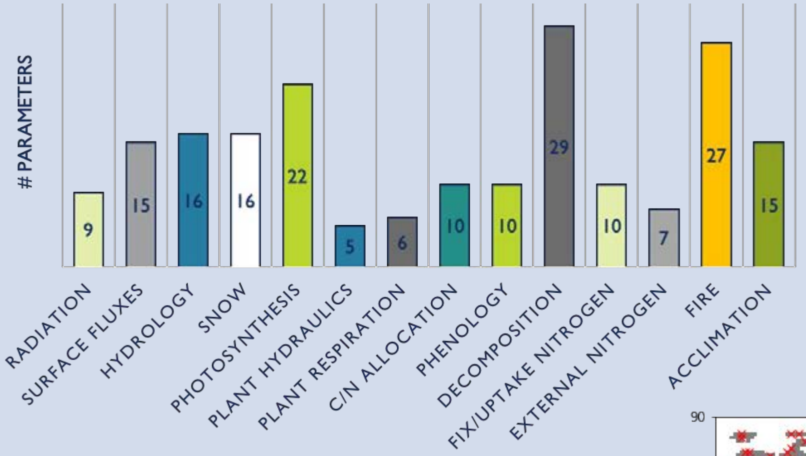
International Land Model Benchmarking (ILAMB) project

- Integrates analysis of ~35 land variables against 90+ 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

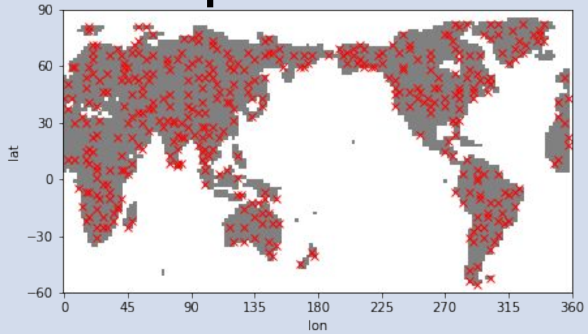
DOE, NCAR, University collaboration

CLM PPE Project

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



Sparse Grid



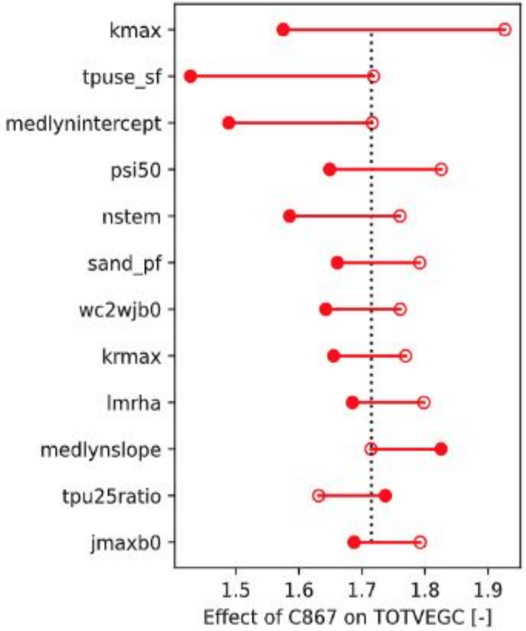
Until recently, computationally prohibitive to attempt to calibrate global CLM(BGC)

- Cluster analysis → reasonably replicate global simulation results with 400 gridcells (Hoffman et al., 2013)
- Matrix solution to C/N initial states decreases spinup timescale by >10X (Lu et al., 2020)

CLM 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
  - Control: present-day climate and CO_2
  - 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



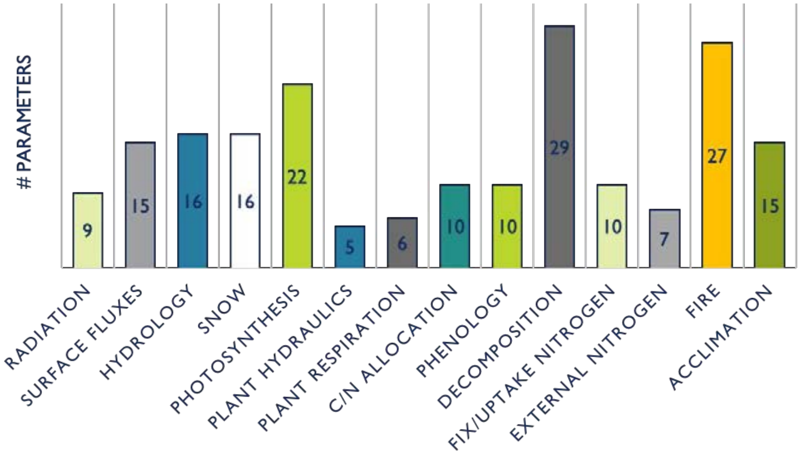
CLM5 Perturbed Parameter Ensemble Project

- **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 (low/high CO_2, PI and future climate, N-dep)

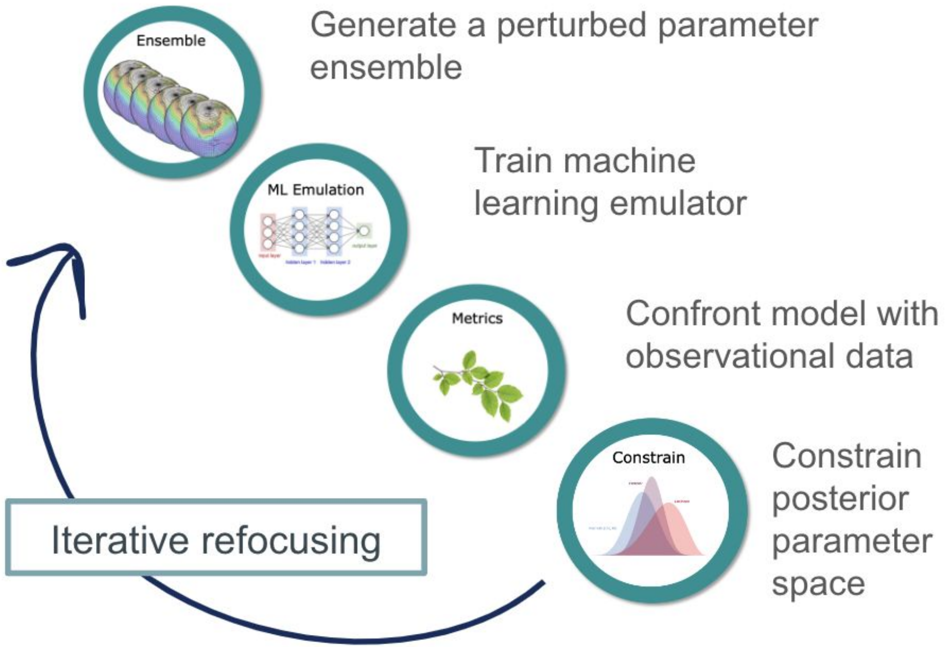
CLM PPE Spinoff Projects

- 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 U)
- …

CLM5 has over 200 parameters



Towards global parameter calibration (testing with LAI calibration)



Important params for Leaf Area Index

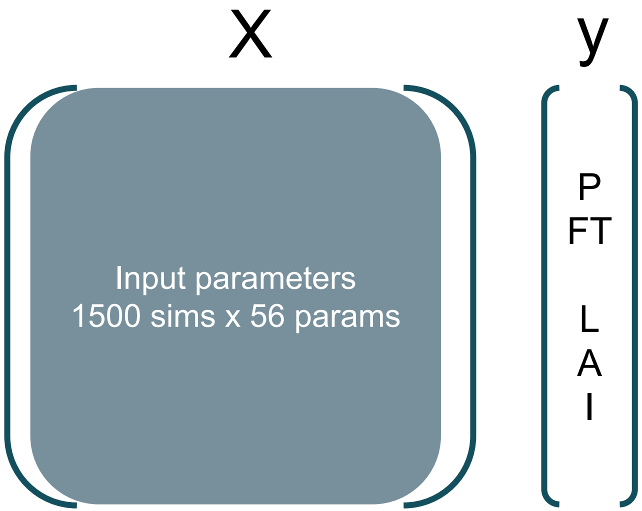
Parameter	Param type
jmaxb0	Photosynthesis
jmaxb1	
wc2wjb0	
theta_cj	
leafcn (PFT)	
jmaxha	
tpu25ratio	
hksat_sf	Soil hydrology
fff	
sucsat_sf	
d_max	
kmax (PFT)	Plant water use
medlynslope (PFT)	
medlynintercept (PFT)	
crit_dayl	Phenology
soilpsi_off	
leaf_long (PFT)	Leaf physiology
slatop (PFT)	
lmr_intercept_atkin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

LEAP

NCAR
UCAR

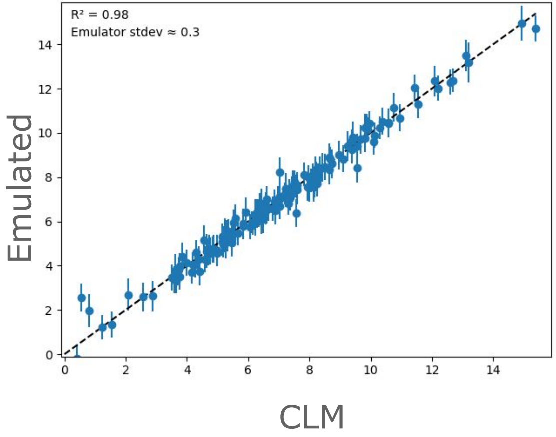
History Matching

Train emulator for each PFT

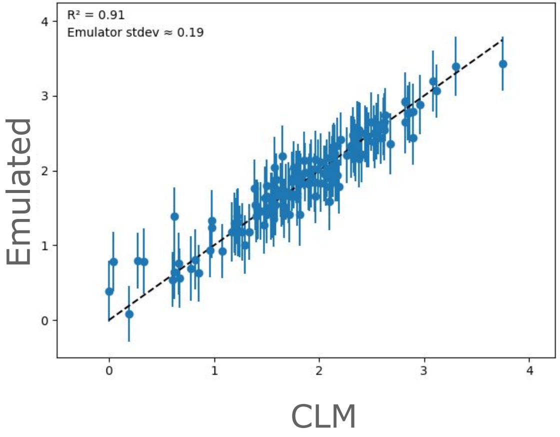


Leaf Area Index

Broadleaf Evergreen Tropical Tree



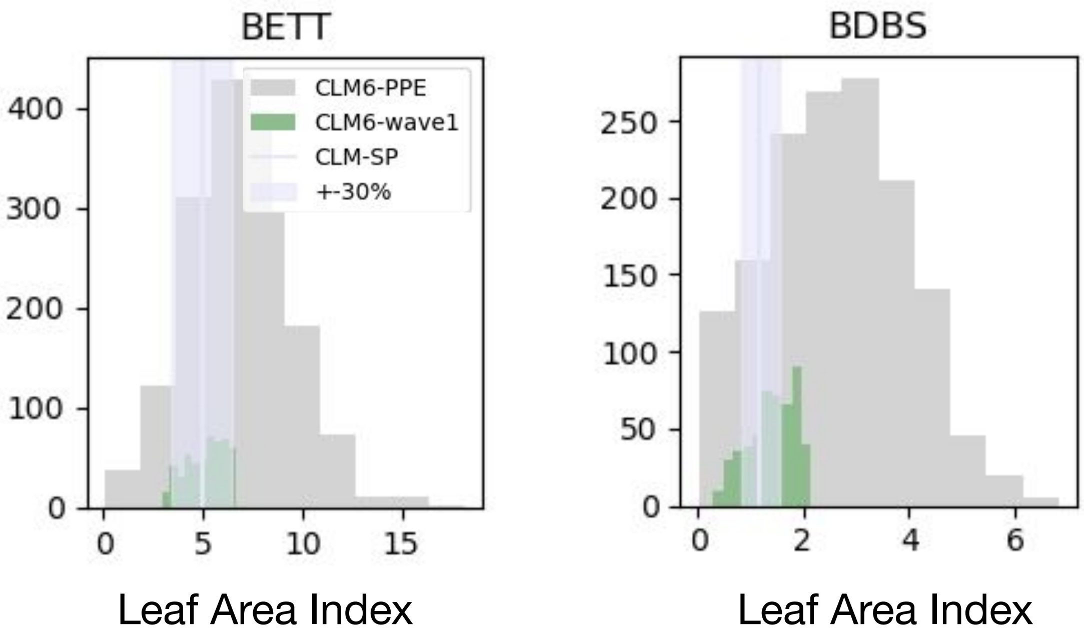
Broadleaf Deciduous Boreal Shrub Tree



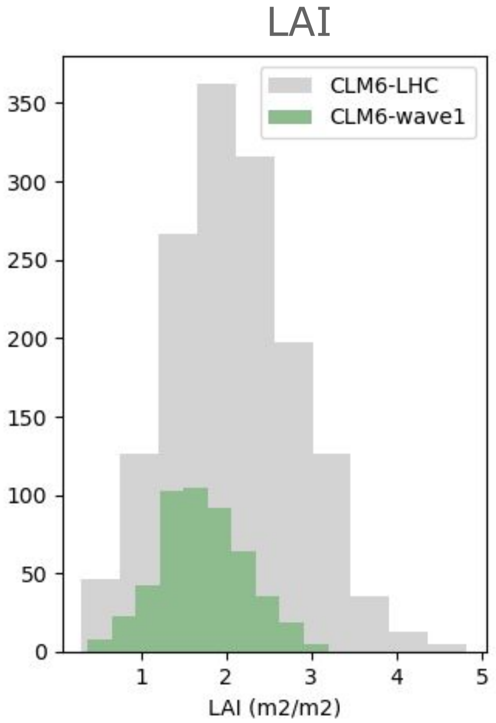
History Matching

Train emulator for each PFT

History Matching
- Sample
- Emulate
- Score (cost function)
- Select best 500 parameter sets



Results *(global mean)*



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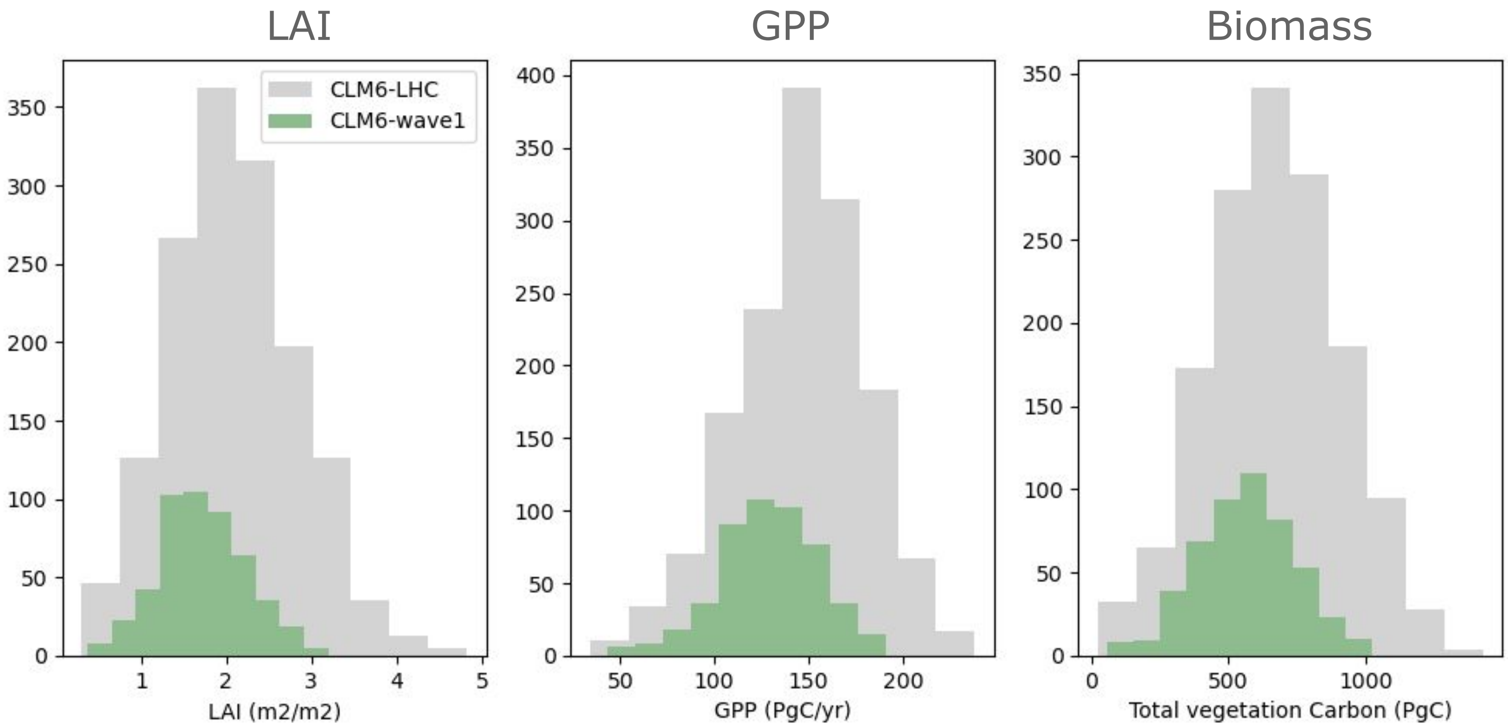

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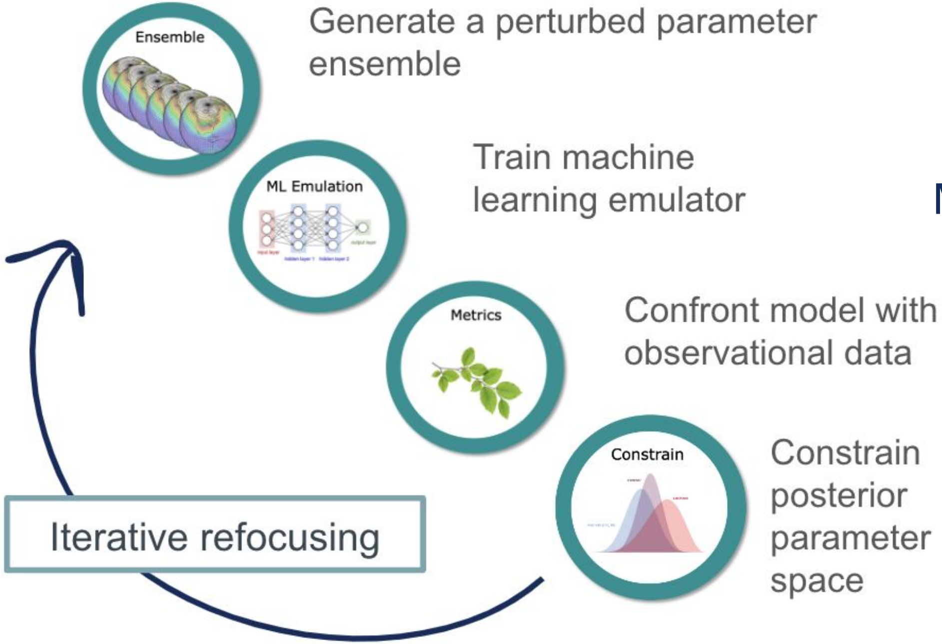
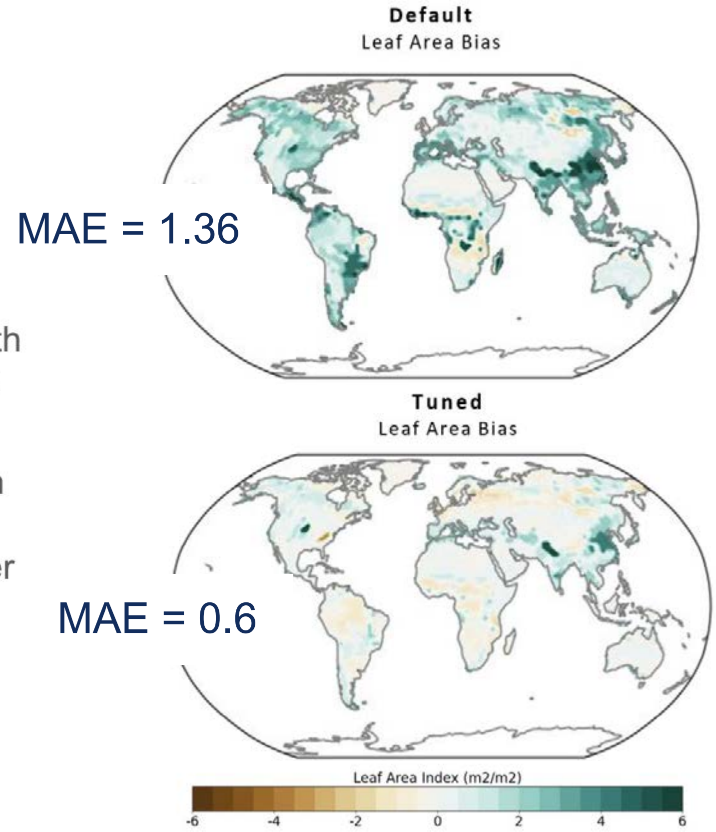
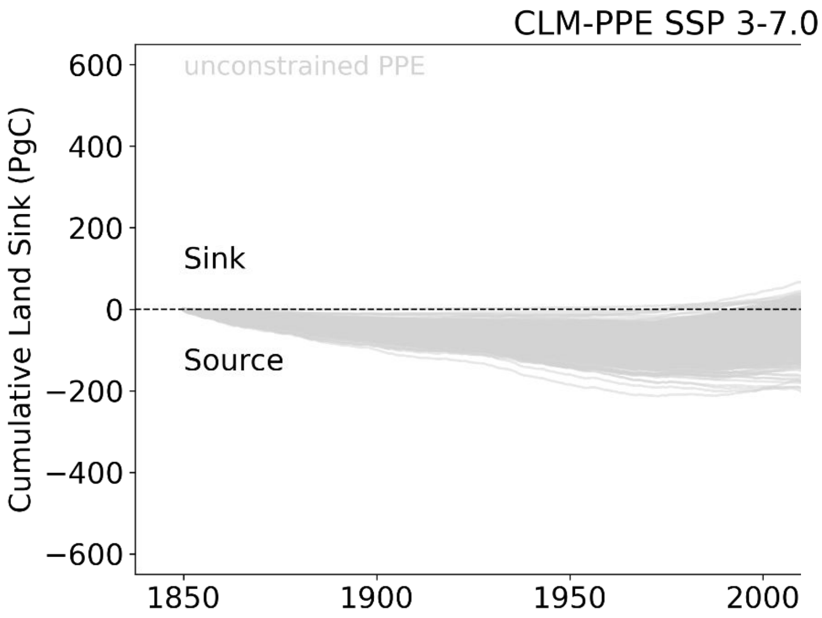




Constraining land carbon cycle projections

500 land-only simulations with Latin Hypercube generated parameter sets (25 parameters)



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theta_cj	
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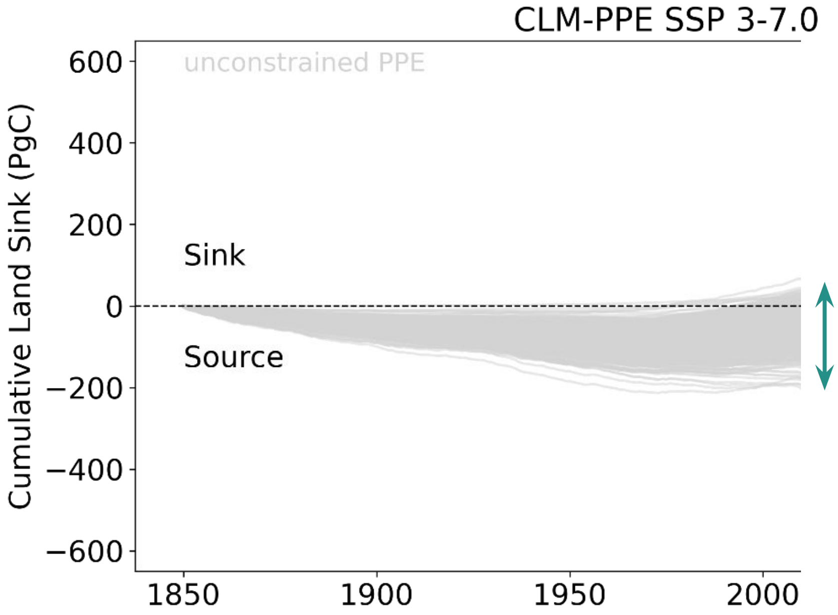
tpu25ratio	
hksat_sf	Soil hydrology
fff	
sucsat_sf	
d_max	
kmax (PFT)	Plant water use
medlynslope (PFT)	
medlynintercept (PFT)	
crit_dayl	Phenology
soilpsi_off	
leaf_long (PFT)	Leaf physiology
slatop (PFT)	
lmr_intercept_atkin	Respiration
lmrha	
froot_leaf (PFT)	Allocation
FUN_fracfixers (PFT)	Nitrogen uptake
pc	Snow

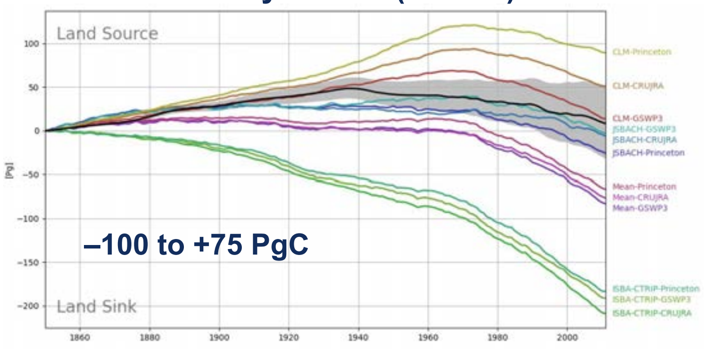
Constraining land carbon cycle projections

500 land-only simulations
with Latin Hypercube generated
parameter sets (25 parameters)



–200 to +50 PgC

Land-only CMIP6 (ILAMB)



Constraining land carbon cycle projections

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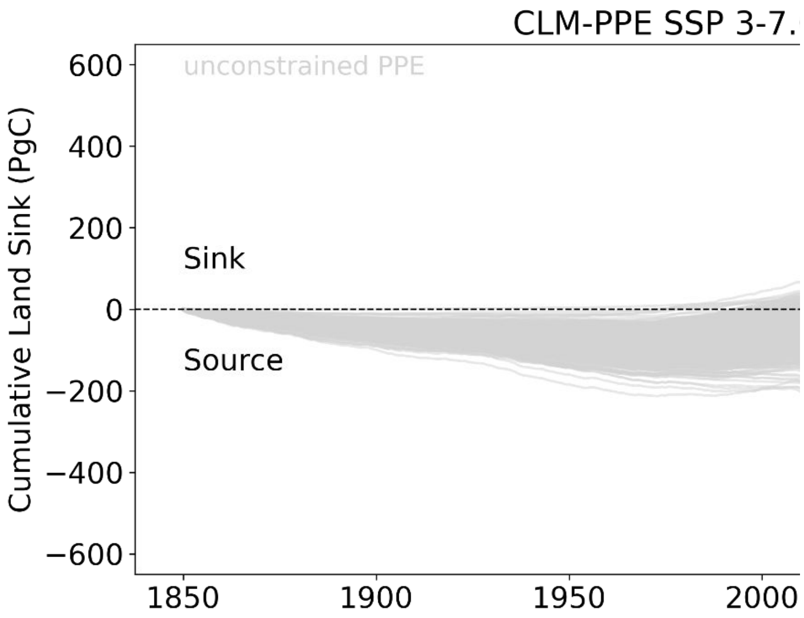
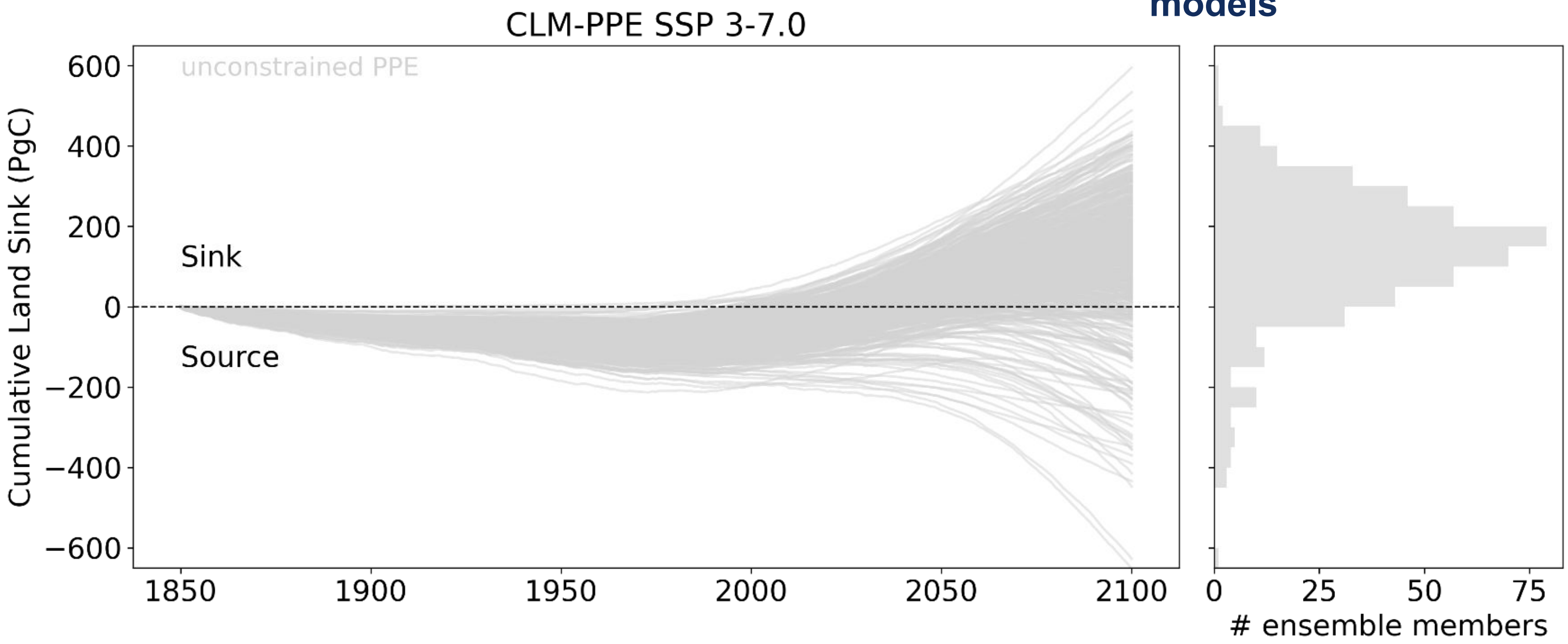


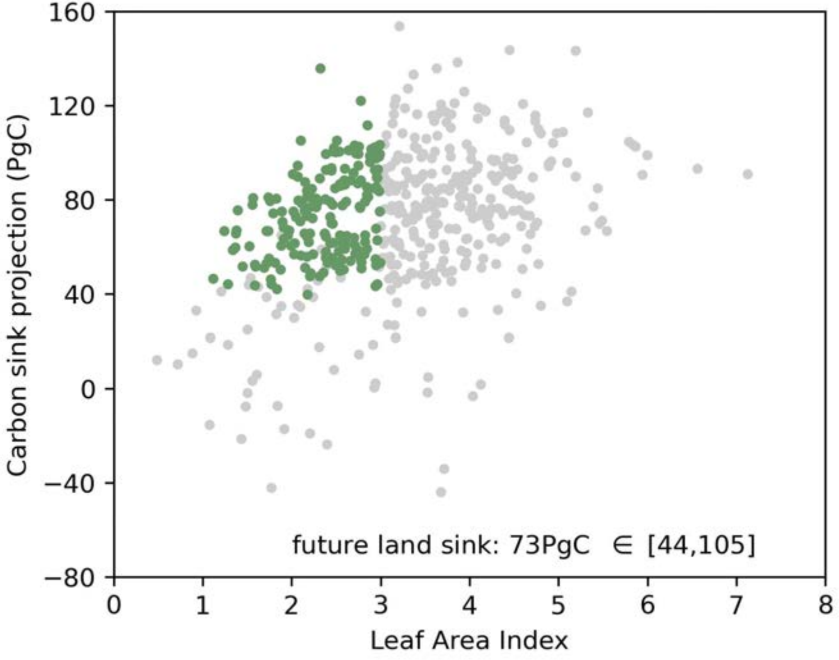
Constraining land carbon cycle projections

500 land-only simulations
with latin hypercube generated
parameter sets (25 parameters)

Range ±600PgC is as large as across CMIP6 models



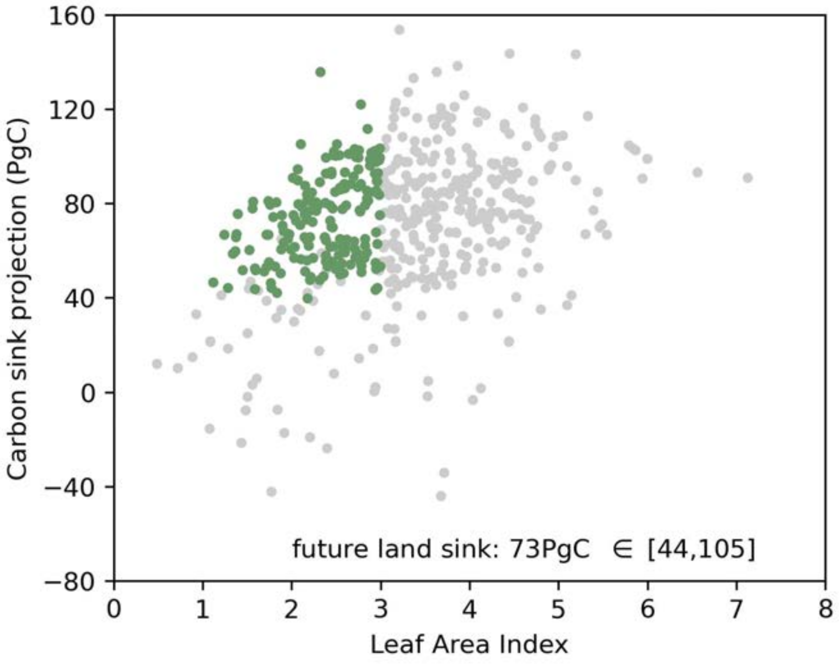
Constraining land carbon cycle projections (history matching)



Can we constrain by retaining only parameter sets with reasonable values for 'observed' quantities?

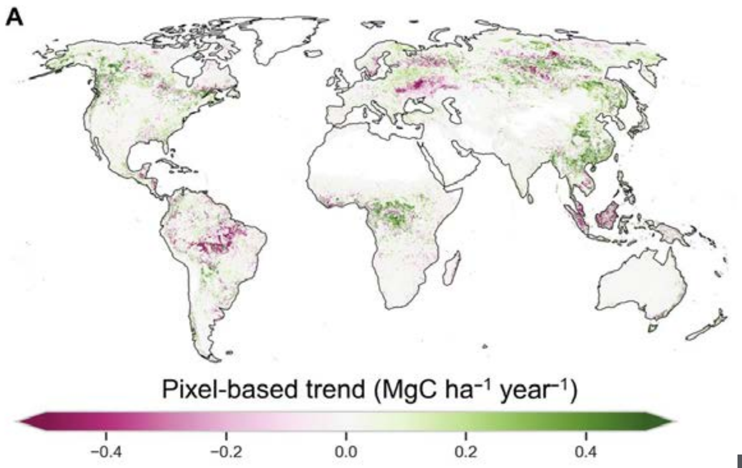
- leaf area index mean / trend

Constraining land carbon cycle projections (history matching)



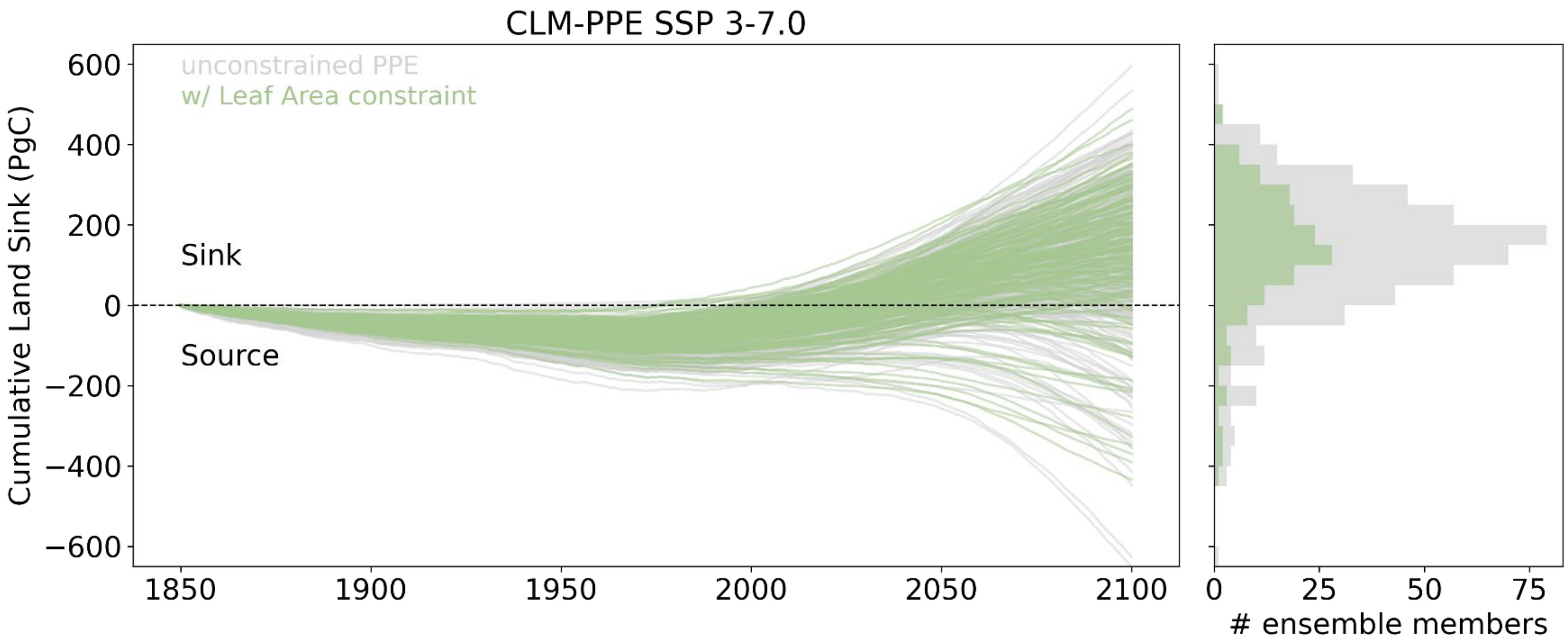
Can we constrain by retaining only parameter sets with reasonable values for ‘observed’ quantities?

- leaf area index mean / trend
- total land use flux (e.g., from bookkeeping models)
- recent changes in live woody biomass from inventories/satellite (Xu et al, 2021)



Constraining land carbon cycle projections

500 land-only simulations
with Latin Hypercube generated
parameter sets (25 parameters)



Constraining land carbon cycle projections

500 land-only simulations
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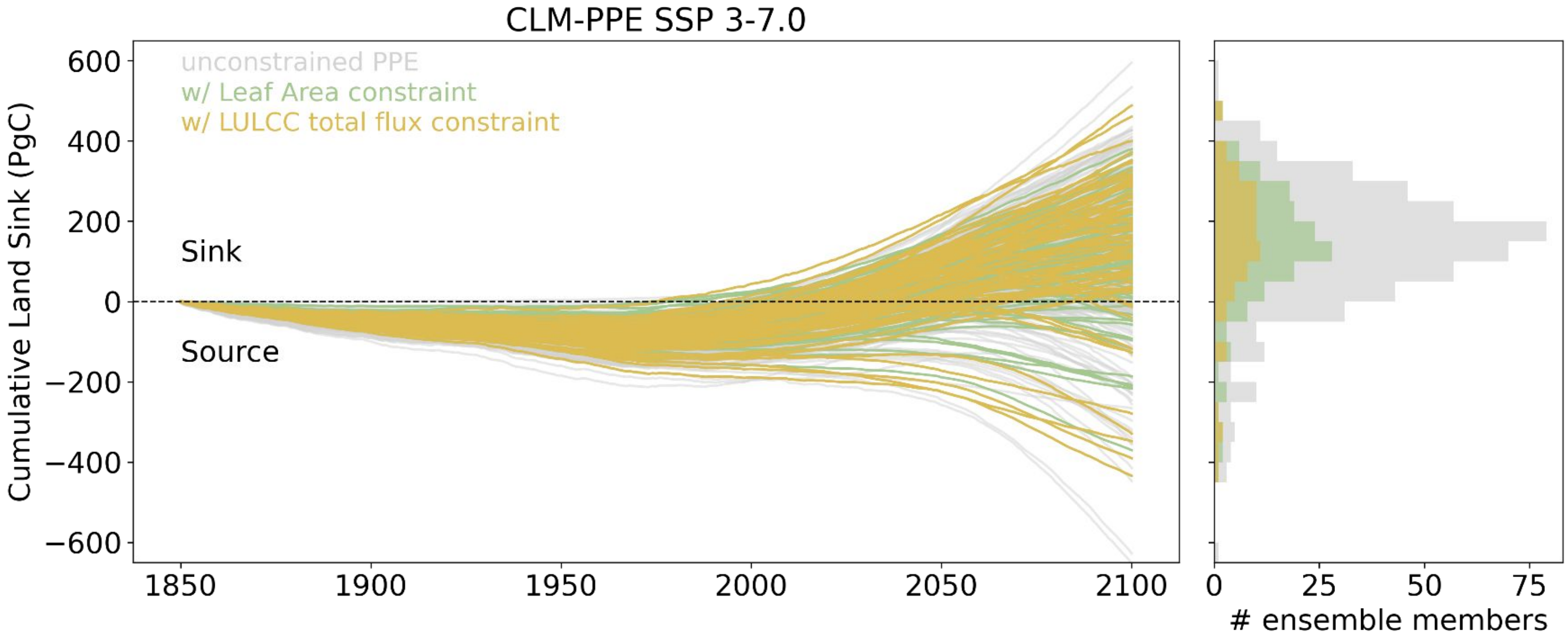

Constraining land carbon cycle projections

500 land-only simulations
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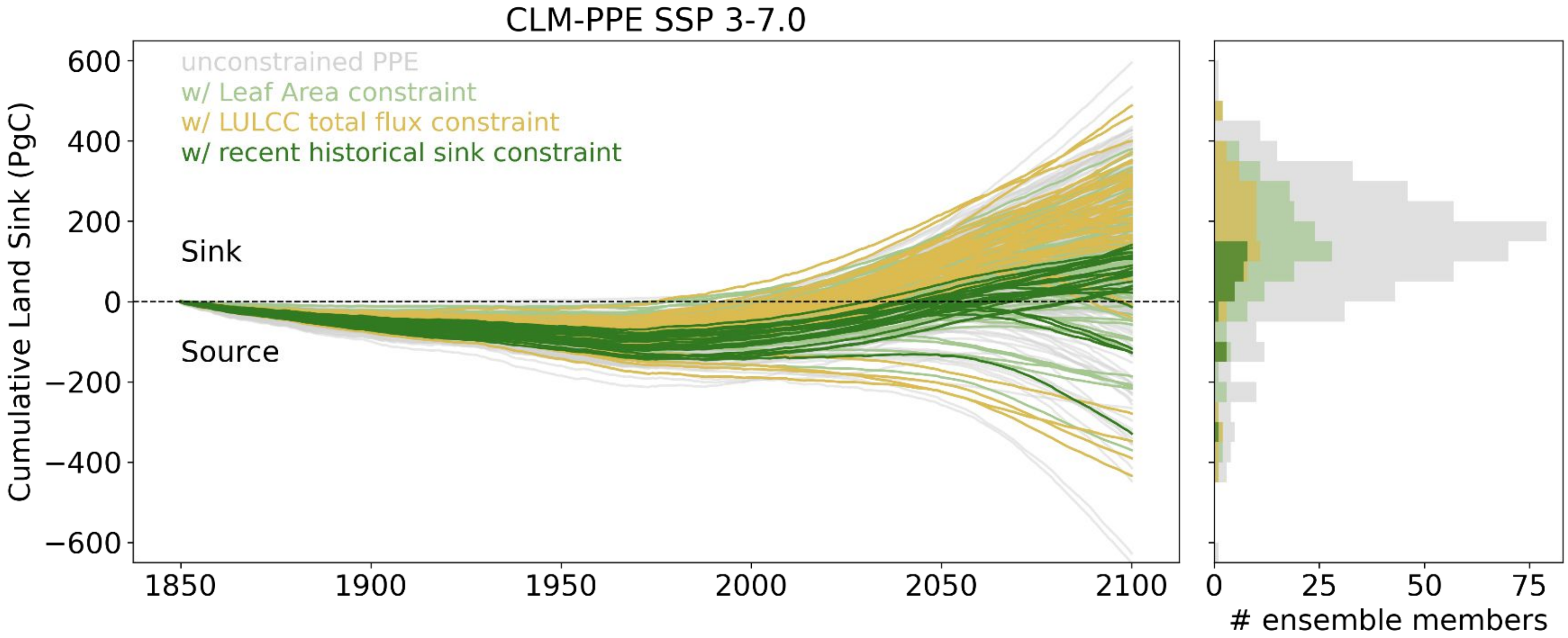
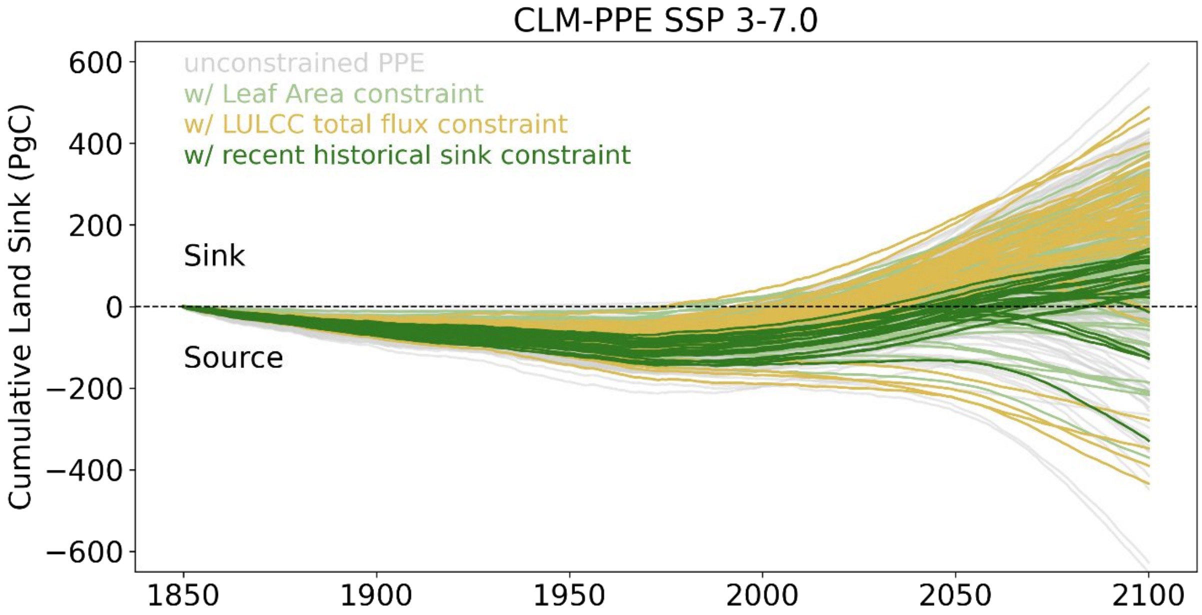


Constraining land carbon cycle projections

500 land-only simulations with Latin Hypercube generated parameter sets (25 parameters)

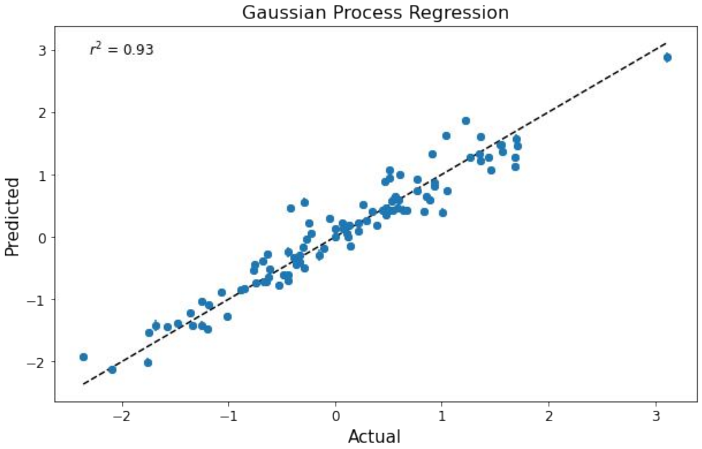


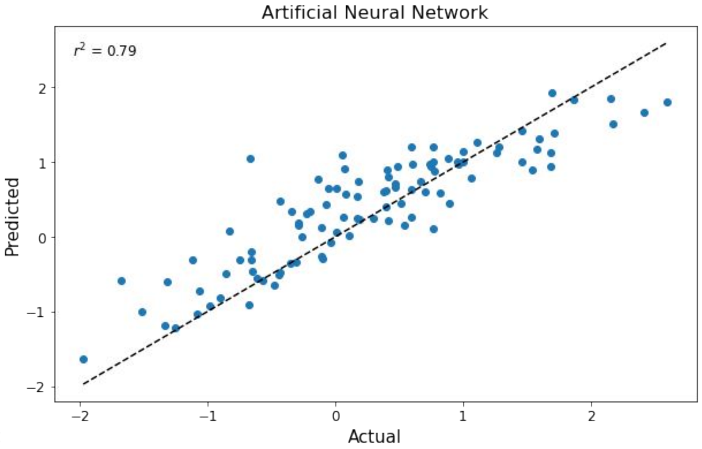
Still a diversity of carbon trend responses, even in constrained sets, but range is much smaller

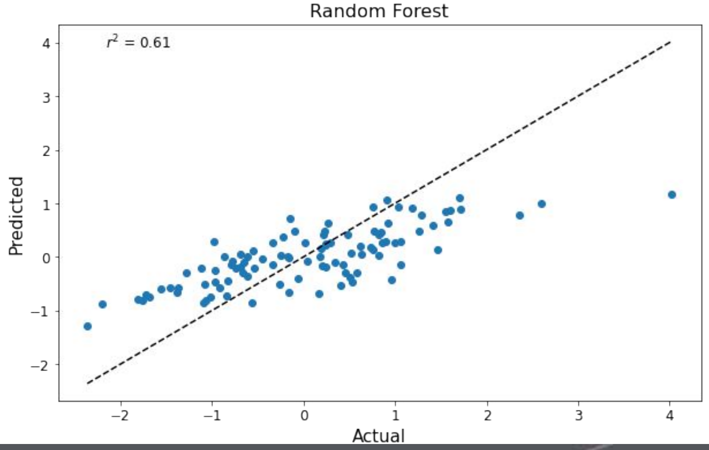
Can we build a future emissions-driven Large Ensemble by including multiple land carbon parameter sets to span this uncertainty as another ensemble dimension (in addition to Initial conditions)?

Parameter Estimation challenges (incomplete list)

Many emulation algorithms with differing performance







Emulating global annual mean leaf area index

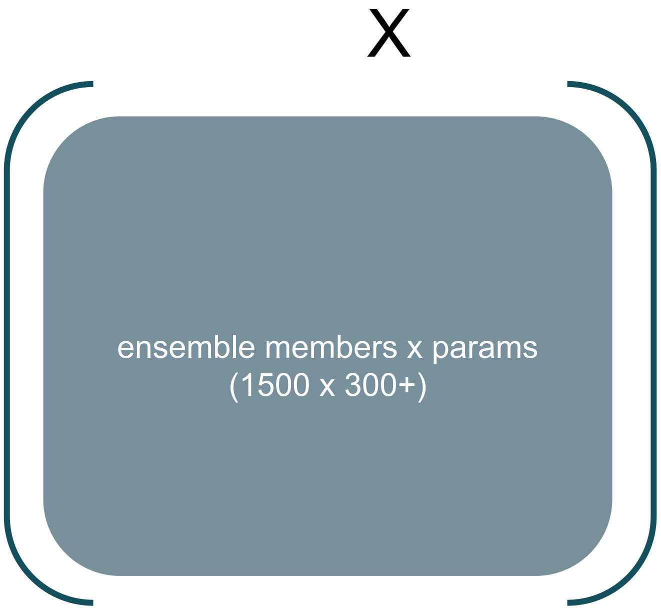
***Preliminary** hyperparameter tuning in progress!*

Thanks to the ESEm Python package:
https://github.com/duncanwp/ESEm
Watson-Parris et al. 2021

Challenges with PFT parameters

To reduce regional biases, need to be able to tune PFT parameters independently

1) Too many parameters (10-15 PFT parameters x 16 PFTs = 300+)



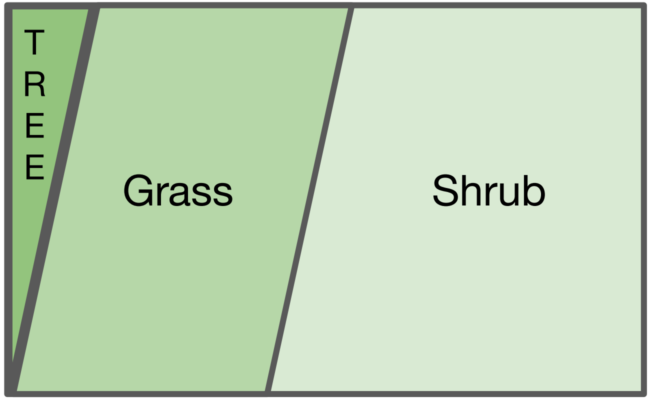
Challenges with PFT parameters

To reduce regional biases, need to be able to tune PFT parameters independently

1) Too many parameters (10-15 PFT parameters x 16 PFTs = 300+)

2) Most observational datasets are not disaggregated by PFT

Fractional PFT coverage in 1 gridcell



Challenge: Coupled vs Land-only parameter impacts

Impact of parameter perturbations can be different in Coupled vs Land-only (offline) simulations, even exhibiting a different sign of response

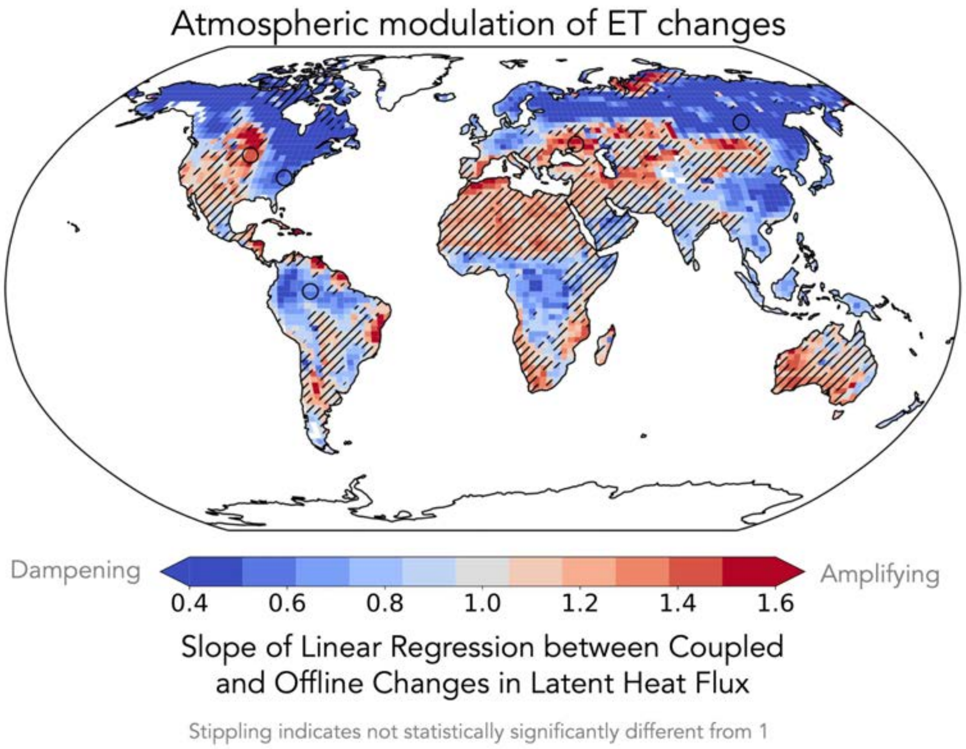


Figure from Zarakas et al., in review

Parameter Estimation challenges (incomplete list)

- As you add constraints (new obs variables and/or constraints beyond means like annual cycle amplitude, interannual variability, trends) → possible to likely that cannot find reasonable parameter sets that meet all constraints → structural errors
- Calibrating the whole model all at once is likely impractical as model complexity rises (e.g., FATES full competition mode)
    - Calibration cascade methodology likely needed

CalLMIP (aimesproject.org/cal-lmip/)

Calibrated Land Model Intercomparison Project (CalLMIP):

Planning & Development Workshop

Virtual Workshop Dates

The workshop will consist of three sessions, each lasting 1.5 hours. To accommodate participants across different time zones, we are offering two time options per session: one for the eastern US/EU time zones and one for the Western US/Australia/Asia time zones.

- Session 1: Thursday, March 6 at 8:00-9:30 pm EST OR Friday, March 7 at 10:00-11:30 am EST (time zone converter)
- Session 2: Wednesday, March 19 at 10:00-11:30 am EDT OR Wednesday, March 19 at 8:00-9:30 pm EDT (time zone converter)
- Session 3: Tuesday, April 1st at 10:00-11:30 am EDT OR Tuesday, April 1st at 8:00-9:30 pm EDT (time zone converter)

Workshop Organizers

Natasha MacBean, Nina Raoult, Natalie Douglas, Jana Kolassa, Tristan Quaife, Istem Fer, Daniel Kennedy, Linnia Hawkins, Katie Dagon, Hannah Liddy

Next-generation Earth System modeling to address urgent mitigation and adaptation needs

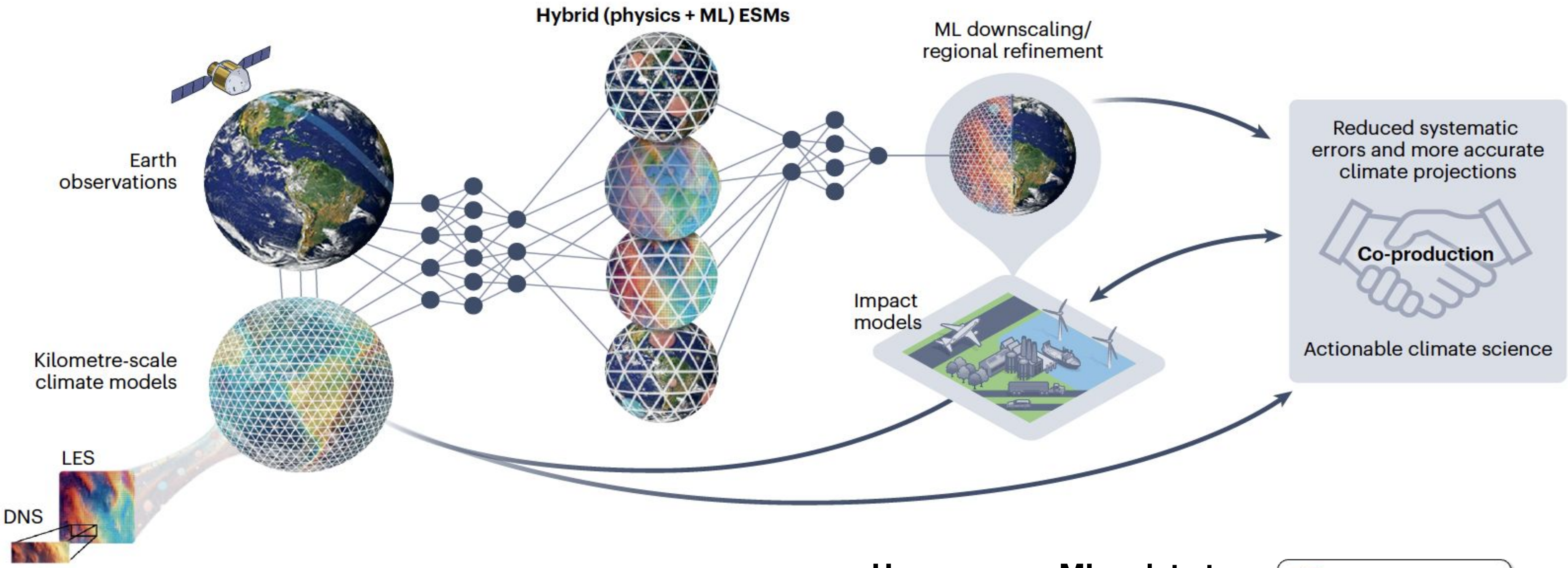


Figure from Eyring, Gentine, Camps-Valls, Lawrence, Reichstein (Nature Climate Change, 2024)

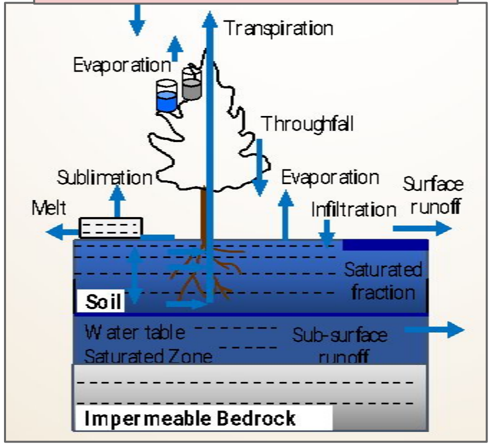
Harness new ML + data to transform ESMs

LEAP forward in the ***reliability***, ***utility***, *and* ***reach*** *of climate projections through synergistic innovations in data science and climate science*

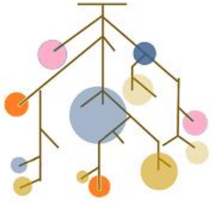
Thank you!

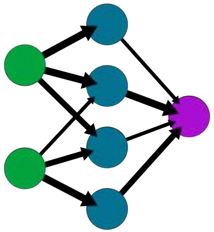
Machine Learning for Land Model Emulation

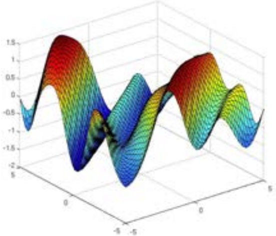
Input: **x number** of land model parameter values



Machine learning emulator *(e.g., neural network, random forest, gaussian process model)*







Output: land **variable/metric** of interest