U.S. DEPARTMENT of ENERGY

Exploiting Artificial Intelligence and Machine Learning to Advance Earth System Science

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University of Tennessee Resource Center, 1201 Oak Ridge Turnpike, Oak Ridge, Tennessee USA

Forrest M. Hoffman, Computational Earth System Scientist

- Group Leader for the ORNL Integrated Computational Earth Sciences Group
- 37 years at ORNL: 15 years in Environmental Sciences Division, 14 years in Computer Science and Mathematics Division, and 8 years in Computational Sciences and Engineering Division
- Develop and apply Earth system models to study global biogeochemical cycles, including terrestrial & marine carbon cycle
- Investigate methods for reconciling uncertainties in carbon–climate feedbacks through comparison with observations
- Apply artificial intelligence methods (machine learning and data mining) to environmental characterization, simulation, & analysis
- Joint Faculty, University of Tennessee, Knoxville, Department of Civil & Environmental Engineering

Oak Ridge National Laboratory

The University of Tennessee Knoxville

Professional Journey Punctuated by Educational Achievements

My academic progress overlapped my career development – “You learn all your life” was taken literally!

Astrophysics | Ecological Modeling | Computer Science | Computational Earth System Science

1983		Dropped out of high school
1986		University of Hawaii Hilo
1988	Self Reinvention	UG Internship at ORNL
1991		BS Physics at UTK
1993		Hired as Research Staff in ESD
2003	Self Reinvention	Transferred to CSMD
2004		MS Physics at UTK
2010	Self Reinvention	1-year Sabbatical to UC Irvine
2012		MS ESS at UC Irvine
2015		PhD ESS at UC Irvine
2016		Joint Faculty at UTK
2017		Transferred to CSED
2020	AAAS (American Association for the Advancement of Science) Fellow; IEEE Senior Member	Group Leader for CESG
2025		Corporate Fellow

Much more work to do!

OAK RIDGE National Laboratory

THE UNIVERSITY OF TENNESSEE
Oak Ridge Innovation Institute

Introduction

- Observations of the Earth system are increasing in spatial resolution and temporal frequency, and will grow exponentially over the next 5–10 years
- With Exascale computing, simulation output is growing even faster, outpacing our ability to analyze, interpret and evaluate model results
- Explosive data growth and the promise of discovery through data-driven modeling necessitate new methods for feature extraction, change/anomaly detection, data assimilation, simulation, and analysis

Frontier at Oak Ridge National Laboratory is the #2 fastest supercomputer on the TOP500 List (Nov 2025) and the first supercomputer to break the exaflop barrier (Jun 2022)

FOCUS | NEXT-GENERATION SUPERCOMPUTERS

This article is the second in a two-part series. The first part, "How to Build a Hypercomputer," by Thomas Sterling, appeared in the July 2001 issue.

The Do-It-Yourself Supercomputer

By William W. Hargrove, Forrest M. Hoffman and Thomas Sterling

Photographs by Kay Chernush

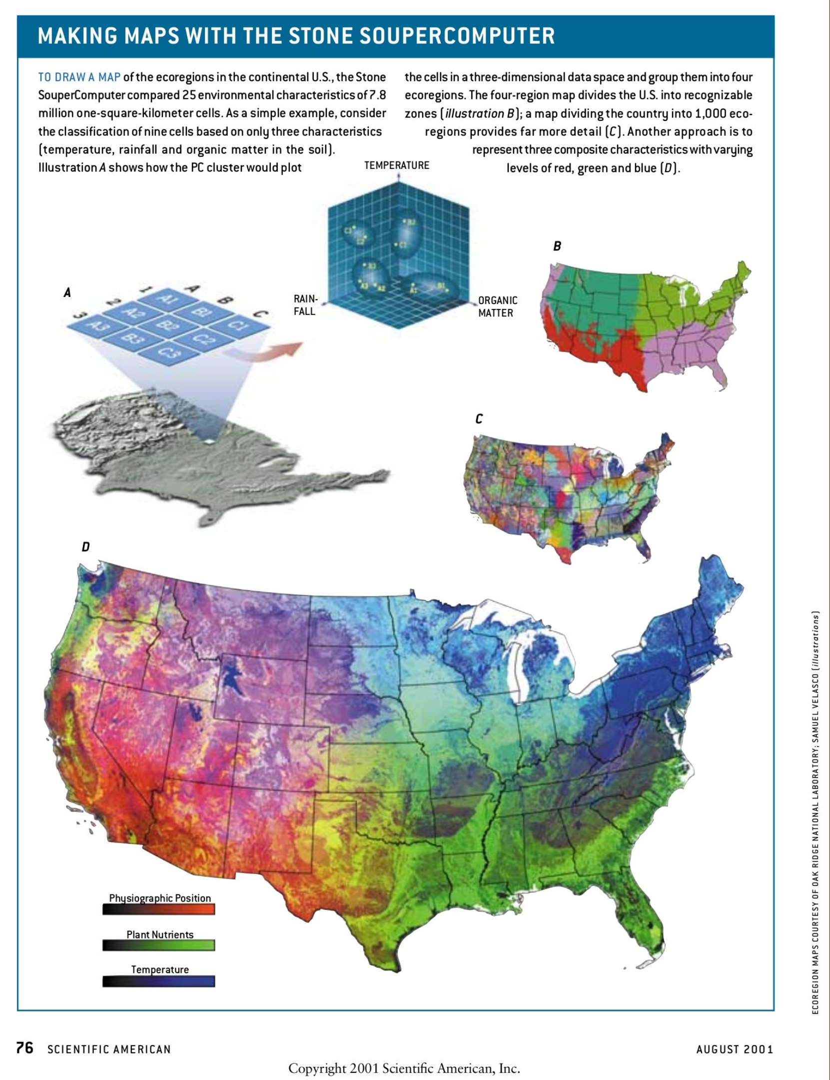
Scientists have found a cheaper way to solve tremendously difficult computational problems: connect ordinary PCs so that they can work together

CLUSTER OF PCs at the Oak Ridge National Laboratory in Tennessee has been dubbed the Stone SouperComputer.

Hargrove, W. W., F. M. Hoffman, and T. Sterling (2001), The Do-It-Yourself Supercomputer, *Sci. Am.*, 265(2):72–79, https://www.scientificamerican.com/article/the-do-it-yourself-superc/

Multivariate Geographic Clustering

- Ecoregions have traditionally been created by experts
- Our approach has been to objectively create ecoregions using continuous continental-scale data and clustering
- We developed a highly scalable *k*-means cluster analysis code that uses distributed memory parallelism
- Originally developed on a 486/Pentium cluster, the code now runs on the largest hybrid CPU/GPU architectures on Earth



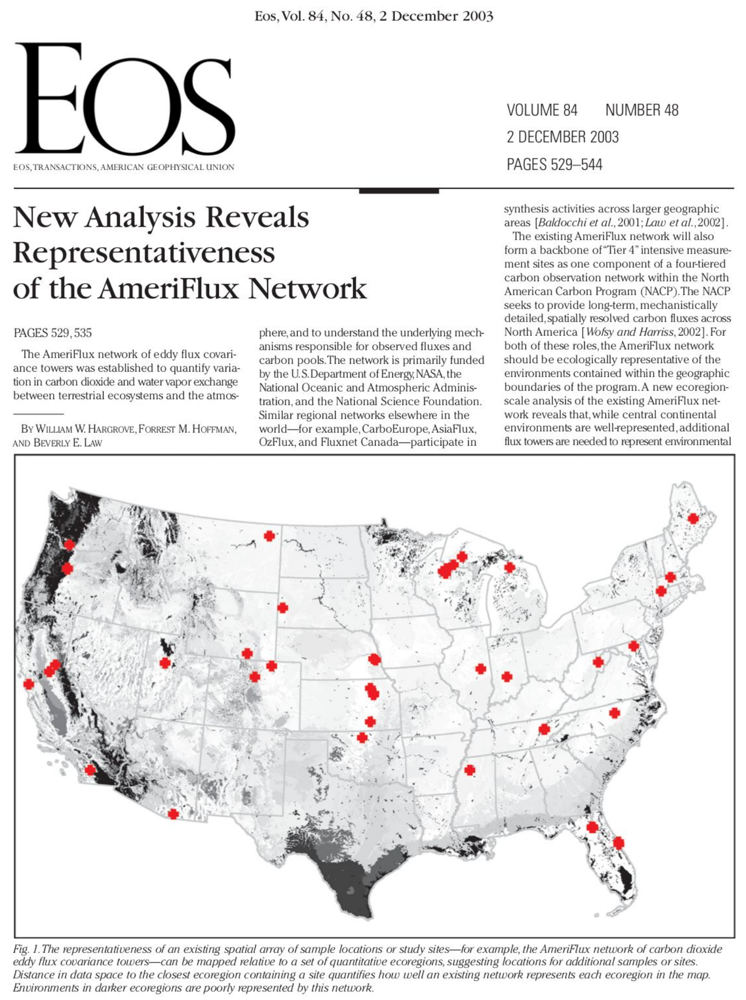
MAKING MAPS WITH THE STONE SOUPERCOMPUTER

TO DRAW A MAP of the ecoregions in the continental U.S., the Stone SouperComputer compared 25 environmental characteristics of 7.8 million one-square-kilometer cells. As a simple example, consider the classification of nine cells based on only three characteristics (temperature, rainfall and organic matter in the soil). Illustration *A* shows how the PC cluster would plot the cells in a three-dimensional data space and group them into four ecoregions. The four-region map divides the U.S. into recognizable zones (*illustration B*); a map dividing the country into 1,000 eco-regions provides far more detail (*C*). Another approach is to represent three composite characteristics with varying levels of red, green and blue (*D*).

ECOREGION MAPS COURTESY OF OAK RIDGE NATIONAL LABORATORY; SAMUEL VELASCO (*illustrations*)

Hargrove, W. W., F. M. Hoffman, and T. Sterling (2001), The Do-It-Yourself Supercomputer, *Sci. Am.*, 265(2):72–79, https://www.scientificamerican.com/article/the-do-it-yourself-superc/

Network Representativeness



Eos, Vol. 84, No. 48, 2 December 2003

EOS

EOS, TRANSACTIONS, AMERICAN GEOPHYSICAL UNION

VOLUME 84 NUMBER 48

2 DECEMBER 2003

PAGES 529–544

New Analysis Reveals Representativeness of the AmeriFlux Network

PAGES 529, 535

The AmeriFlux network of eddy flux covariance towers was established to quantify variation in carbon dioxide and water vapor exchange between terrestrial ecosystems and the atmosphere, and to understand the underlying mechanisms responsible for observed fluxes and carbon pools. The network is primarily funded by the U.S. Department of Energy, NASA, the National Oceanic and Atmospheric Administration, and the National Science Foundation. Similar regional networks elsewhere in the world—for example, CarboEurope, AsiaFlux, OzFlux, and Fluxnet Canada—participate in synthesis activities across larger geographic areas [*Baldocchi et al.*, 2001; *Law et al.*, 2002].

The existing AmeriFlux network will also form a backbone of "Tier 4" intensive measurement sites as one component of a four-tiered carbon observation network within the North American Carbon Program (NACP). The NACP seeks to provide long-term, mechanistically detailed, spatially resolved carbon fluxes across North America [*Wofsy and Harriss*, 2002]. For both of these roles, the AmeriFlux network should be ecologically representative of the environments contained within the geographic boundaries of the program. A new ecoregion-scale analysis of the existing AmeriFlux network reveals that, while central continental environments are well-represented, additional flux towers are needed to represent environmental

By William W. Hargrove, Forrest M. Hoffman, and Beverly E. Law

Fig. 1. The representativeness of an existing spatial array of sample locations or study sites—for example, the AmeriFlux network of carbon dioxide eddy flux covariance towers—can be mapped relative to a set of quantitative ecoregions, suggesting locations for additional samples or sites. Distance in data space to the closest ecoregion containing a site quantifies how well an existing network represents each ecoregion in the map. Environments in darker ecoregions are poorly represented by this network.

- The *n*-dimensional space formed by the data layers offers a natural framework for estimating representativeness of individual sampling sites
- The Euclidean distance between individual sites in data space is a metric of similarity or dissimilarity
- Representativeness across multiple sampling sites can be combined to produce a map of network representativeness

Hargrove, W. W., and F. M. Hoffman (2003), New Analysis Reveals Representativeness of the AmeriFlux Network, *Eos Trans. AGU*, 84(48):529, 535, doi:10.1029/2003EO480001.

Optimizing Sampling Networks

- Our group produced this network representativeness map for the authors from global climate, edaphic, and elevation and topography data
- Dark areas, including most of the Indian subcontinent, were poorly represented by the constellation of eddy covariance flux towers participating in FLUXNET in the year 2007

Sundareshwar, P. V., et al. (2007), Environmental Monitoring Network for India, *Science*, 316(5822):204–205, doi:[10.1126/science.1137417](https://doi.org/10.1126/science.1137417).

POLICYFORUM

CORRECTED 8 JUNE 2007; SEE LAST PAGE

ENVIRONMENT

Environmental Monitoring Network for India

An integrated monitoring system is proposed for India that will monitor terrestrial, coastal, and oceanic environments.

P. V. Sundareshwar,* R. Murtugudde, G. Srinivasan, S. Singh, K. J. Ramesh, R. Ramesh, S. B. Verma, D. Agarwal, D. Baldocchi, C. K. Baru, K. K. Baruah, G. R. Chowdhury, V. K. Dadhwal, C. B. S. Dutt, J. Fuentes, Prabhat K. Gupta, W. W. Hargrove, M. Howard, C. S. Jha, S. Lal, W. K. Michener, A. P. Mitra, J. T. Morris, R. R. Myneni, M. Naja, R. Nemani, R. Purvaja, S. Raha, S. K. Santhana Vanan, M. Sharma, A. Subramaniam, R. Sukumar, R. R. Twilley, P. R. Zimmerman

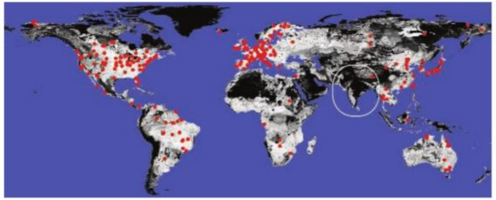
Understanding the consequences of global environmental change and its mitigation will require an integrated global effort of comprehensive long-term data collection, synthesis, and action (1). The last decade has seen a dramatic global increase in the number of networked monitoring sites. For example, FLUXNET is a global collection of >300 micrometeorological terrestrial-flux research sites (see figure, right) that monitor fluxes of CO_2, water vapor, and energy (2–4). A similar, albeit sparser, network of ocean observation sites is quantifying the fluxes of greenhouse gases (GHGs) from oceans and their role in the global carbon cycle (5, 6). These networks are operated on an ad hoc basis by the scientific community. Although FLUXNET and other observation networks cover diverse vegetation types within a 70°S to 30°N latitude band (3) and different oceans (5, 6), there are not comprehensive and reliable data from African and Asian regions. Lack of robust scientific data from these regions of the world is a serious impediment to efforts to understand and mitigate impacts of climate and environmental change (5, 7).

The Indian subcontinent and the surrounding seas, with more than 1.3 billion people and unique natural resources, have a significant impact on the regional and global environment but lack a comprehensive environmental observation network. Within the government of India, the Department of Science and Technology (DST) has proposed filling this gap by establishing INDOFLUX, a coordinated multidisciplinary environmental monitoring network that integrates terrestrial, coastal, and oceanic environments (see figure, right).

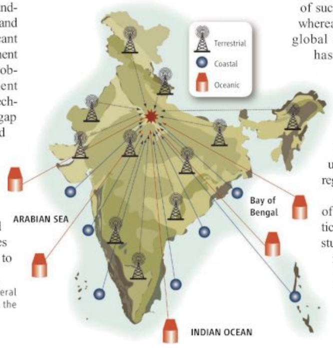
In a workshop held in July 2006 (8), a team of scientists from India and the United States developed the overarching objectives for the proposed INDOFLUX. These are to provide a scientific understanding (i) of the coupling of atmospheric, oceanic, and terrestrial environments in India; (ii) of the nature and pace of environmental change in India; and (iii) of subsequent impacts on provision of ecosystem services. Also, in order to evaluate what will enable India to sustain its natural resources, these goals include an assessment of the vulnerability and consequent risks to its social and natural systems.

Climate change will alter the regional biosphere-climate feedbacks and land-ocean coupling. Although global models reliably predict the trend in the impact of climate change on India's forest resources, the magnitude of such change is uncertain (9). Similarly, whereas all oceans show the influence of global warming (10), the Indian Ocean has shown higher-than-average surface warming, especially during the last five decades (11, 12). This warming may have global impacts (13, 14), even though the impact on the Indian summer monsoons is not well understood (15, 16). These uncertainties highlight the need for regional models driven by regional data.

As the hypoxia observed in the Gulf of Mexico is related to agricultural practices in the watershed (17), Indian Ocean studies also indicate couplings between mainland activities and offshore and



Current monitoring sites in FLUXNET. Sites are shown in red, and global representativeness is estimated by Global Multivariate Clustering Analysis (24–26). Darker areas are poorly represented by the existing FLUXNET towers. Environmental similarity was calculated from a set of variables (precipitation, temperature, solar flux, total soil carbon and nitrogen, bulk density, elevation, and compound topographic index) at a resolution of 4 km.



A schematic of the INDOFLUX proposal. Placement of stations reflects different climactic, vegetation, and land-use areas. Final locations will be determined as part of the formal science plan.

The authors were members of an Indo–U.S. bilateral workshop on INDOFLUX. Affiliations are provided in the supporting online material.

*Author for correspondence. E-mail: pvs@sdsmt.edu

CREDITS (TOP TO BOTTOM): W. W. HARGROVE/P. V. SUNDARESHWAR (SOURCE)

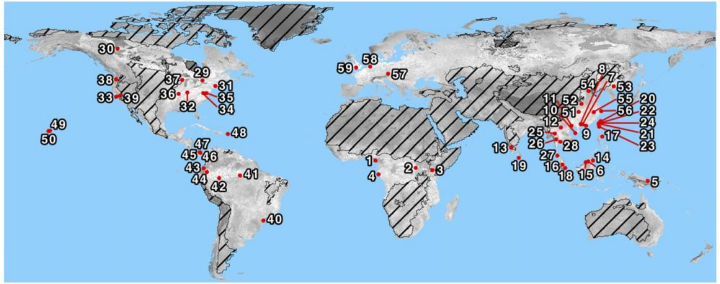


Fig. 1 Map of the CTFS-ForestGEO network illustrating its representation of bioclimatic, edaphic, and topographic conditions globally. Site numbers correspond to ID# in Table 2. Shading indicates how well the network of sites represents the suite of environmental factors included in the analysis; light-colored areas are well-represented by the network, while dark colored areas are poorly represented. Stippling covers nonforest areas. The analysis is described in Appendix S1.

Table 1 Attributes of a CTFS-ForestGEO census

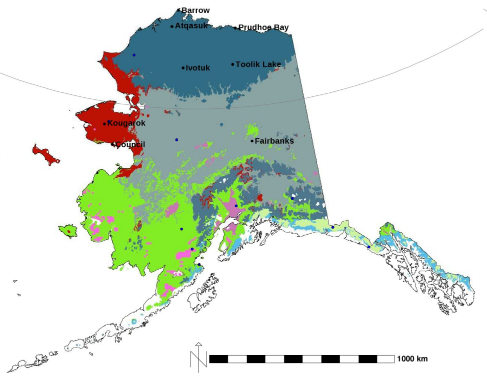
Attribute	Utility
Very large plot size	Resolve community and population dynamics of highly diverse forests with many rare species with sufficient sample sizes (Losos & Leigh, 2004; Condit *et al.*, 2006); quantify spatial patterns at multiple scales (Condit *et al.*, 2000; Wiegand *et al.*, 2007a,b; Detto & Muller-Landau, 2013; Lutz *et al.*, 2013); characterize gap dynamics (Feeley *et al.*, 2007b); calibrate and validate remote sensing and models, particularly those with large spatial grain (Mascaro *et al.*, 2011; Réjou-Méchain *et al.*, 2014)
Includes every freestanding woody stem ≥1 cm DBH	Characterize the abundance and diversity of understory as well as canopy trees; quantify the demography of juveniles (Condit, 2000; Muller-Landau *et al.*, 2006a,b).
All individuals identified to species	Characterize patterns of diversity, species-area, and abundance distributions (Hubbell, 1979, 2001; He & Legendre, 2002; Condit *et al.*, 2005; John *et al.*, 2007; Shen *et al.*, 2009; He & Hubbell, 2011; Wang *et al.*, 2011; Cheng *et al.*, 2012); test theories of competition and coexistence (Brown *et al.*, 2013); describe poorly known plant species (Gereau & Kenfack, 2000; Davies, 2001; Davies *et al.*, 2001; Sonké *et al.*, 2002; Kenfack *et al.*, 2004, 2006)
Diameter measured on all stems	Characterize size-abundance distributions (Muller-Landau *et al.*, 2006b; Lai *et al.*, 2013; Lutz *et al.*, 2013); combine with allometries to estimate whole-ecosystem properties such as biomass (Chave *et al.*, 2008; Valencia *et al.*, 2009; Lin *et al.*, 2012; Ngo *et al.*, 2013; Muller-Landau *et al.*, 2014)
Mapping of all stems and fine-scale topography	Characterize the spatial pattern of populations (Condit, 2000); conduct spatially explicit analyses of neighborhood influences (Condit *et al.*, 1992; Hubbell *et al.*, 2001; Uriarte *et al.*, 2004, 2005; Rüger *et al.*, 2011, 2012; Lutz *et al.*, 2014); characterize microhabitat specificity and controls on demography, biomass, etc. (Harms *et al.*, 2001; Valencia *et al.*, 2004; Chuyong *et al.*, 2011); align on the ground and remote sensing measurements (Asner *et al.*, 2011; Mascaro *et al.*, 2011).
Census typically repeated every 5 years	Characterize demographic rates and changes therein (Russo *et al.*, 2005; Muller-Landau *et al.*, 2006a,b; Feeley *et al.*, 2007a; Lai *et al.*, 2013; Stephenson *et al.*, 2014); characterize changes in community composition (Losos & Leigh, 2004; Chave *et al.*, 2008; Feeley *et al.*, 2011; Swenson *et al.*, 2012; Chisholm *et al.*, 2014); characterize changes in biomass or productivity (Chave *et al.*, 2008; Banin *et al.*, 2014; Muller-Landau *et al.*, 2014)

Optimizing Sampling Networks

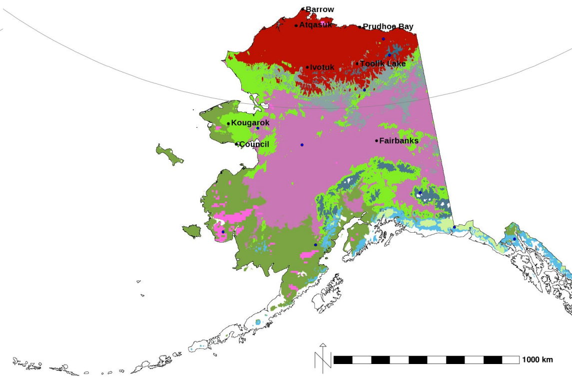
- The CTFS-ForestGEO global forest monitoring network is aimed at characterizing forest responses to global change
- The figure at left shows the global representativeness of the CTFS-ForestGEO sites in 2014
- Non-forested areas are masked with hatching, and as expected, they are consistently darker than the forested regions, which are represented to varying degrees by the monitoring sites

Anderson-Teixeira, K. J., et al. (2015), CTFS-ForestGEO: A Worldwide Network Monitoring Forests in an Era of Global Change, *Glob. Change Biol.*, 21(2):528–549, doi:10.1111/gcb.12712.

Sampling Network Design

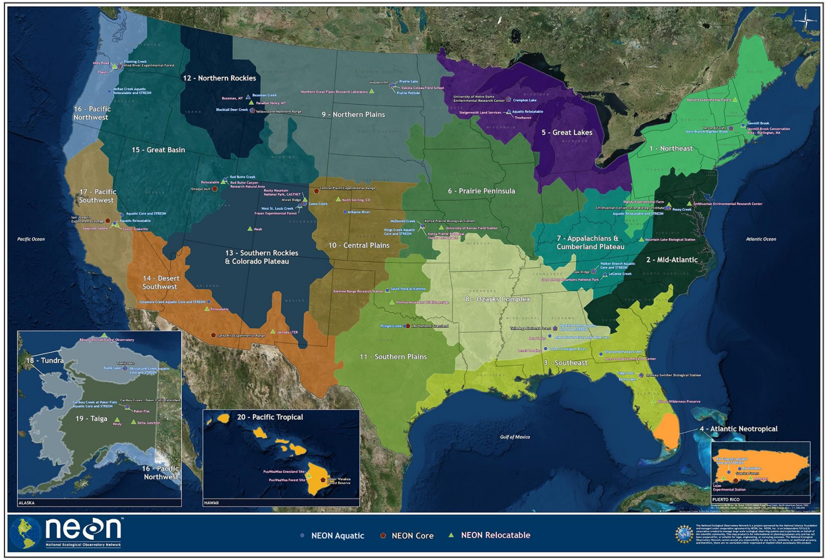


2000–2009



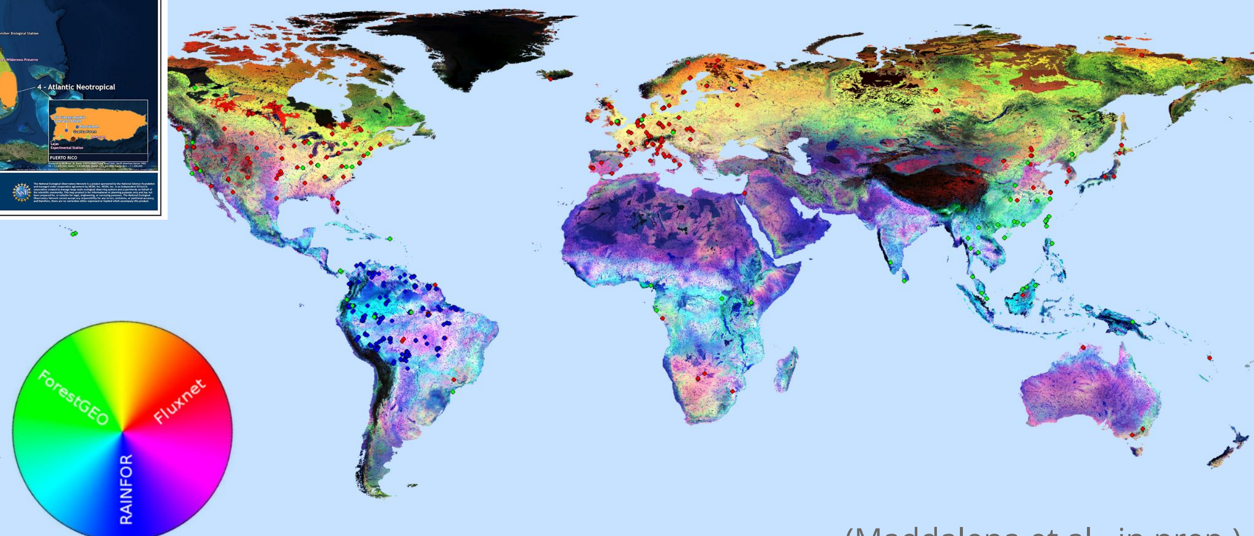
2090–2000

(Hoffman et al., 2013)



NSF's NEON Sampling Domains

Triple-Network Global Representativeness

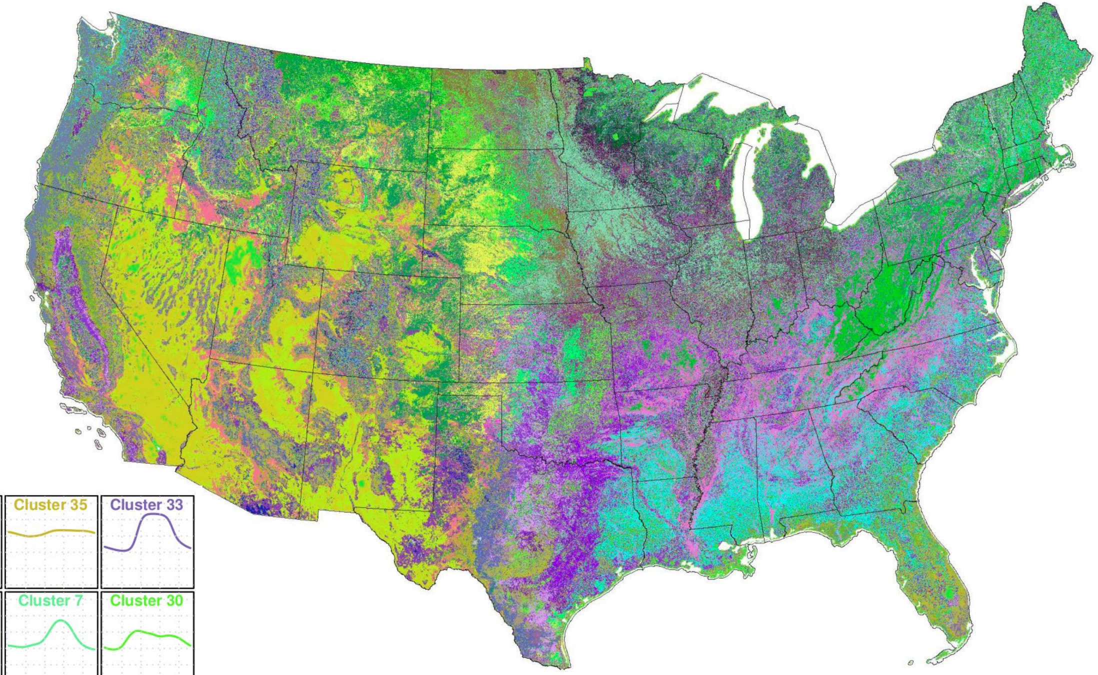


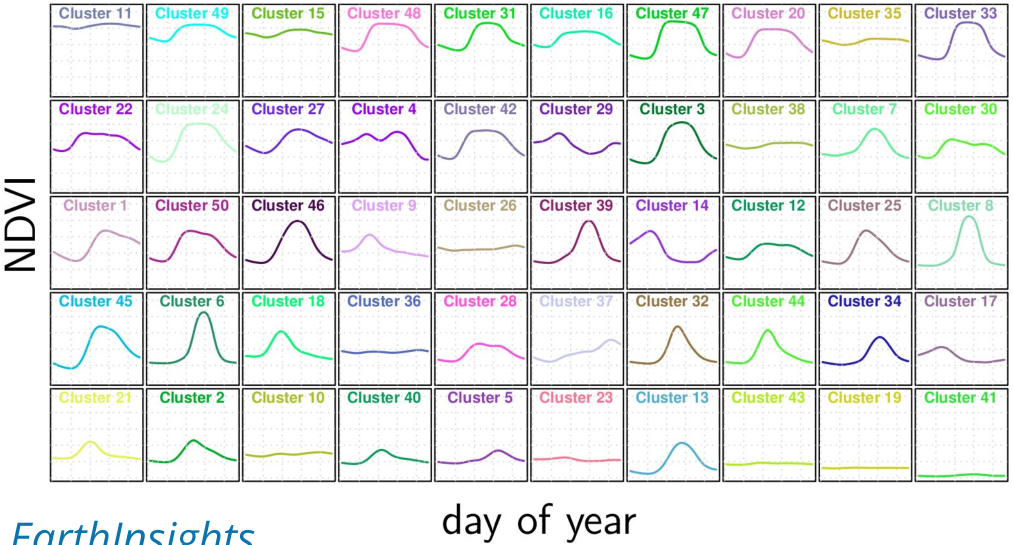
Gridded data from satellite and airborne remote sensing, models, and synthesis products can be combined to design optimal sampling networks and understand representativeness as it evolves through time

(Maddalena et al., in prep.)

50 Phenoregions for year 2012 (Random Colors)

250m MODIS NDVI
Every 8 days (46 images/year)
Clustered from year 2000 to present



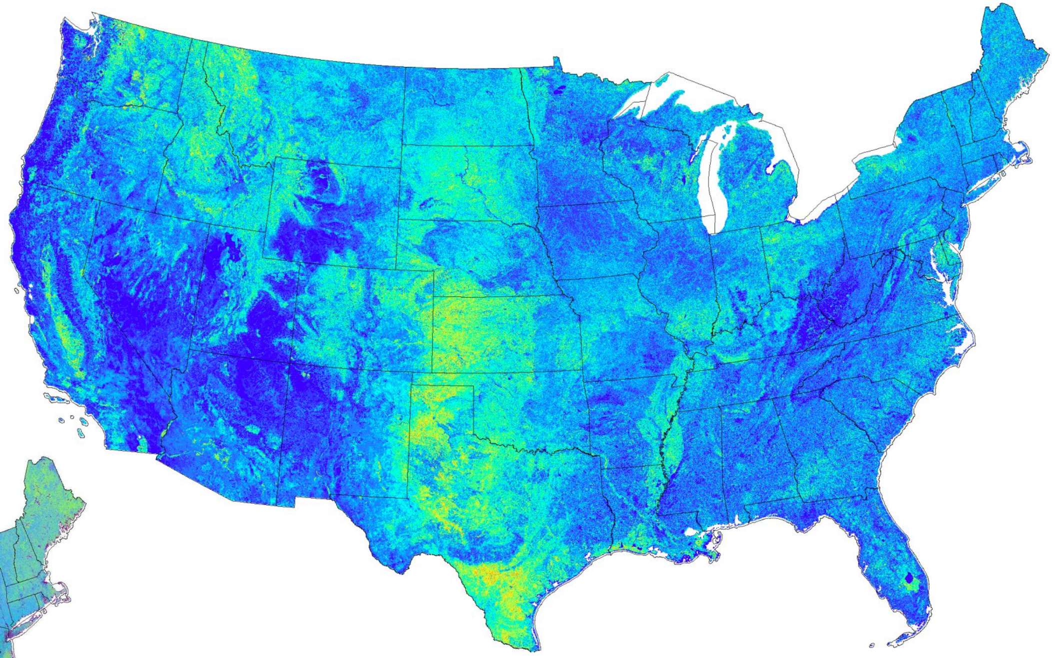


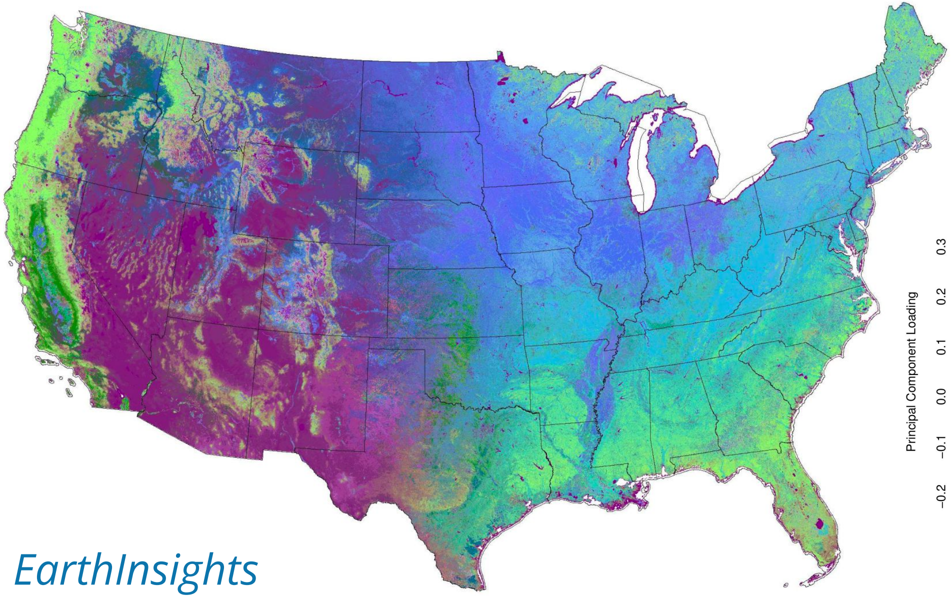
50 Phenoregion Prototypes (Random Colors)

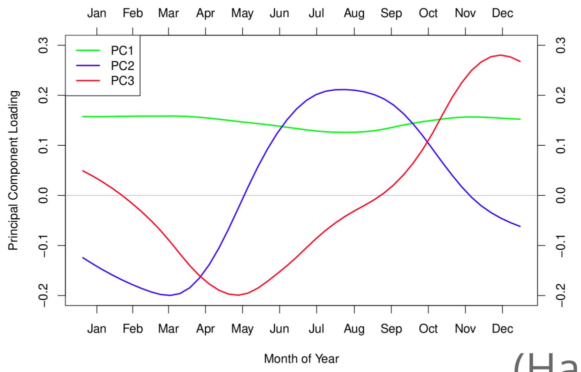
EarthInsights

(Hargrove et al., in prep.)

50 Phenoregions Persistence
and
50 Phenoregions Max Mode
(Similarity Colors)







Principal Components Analysis

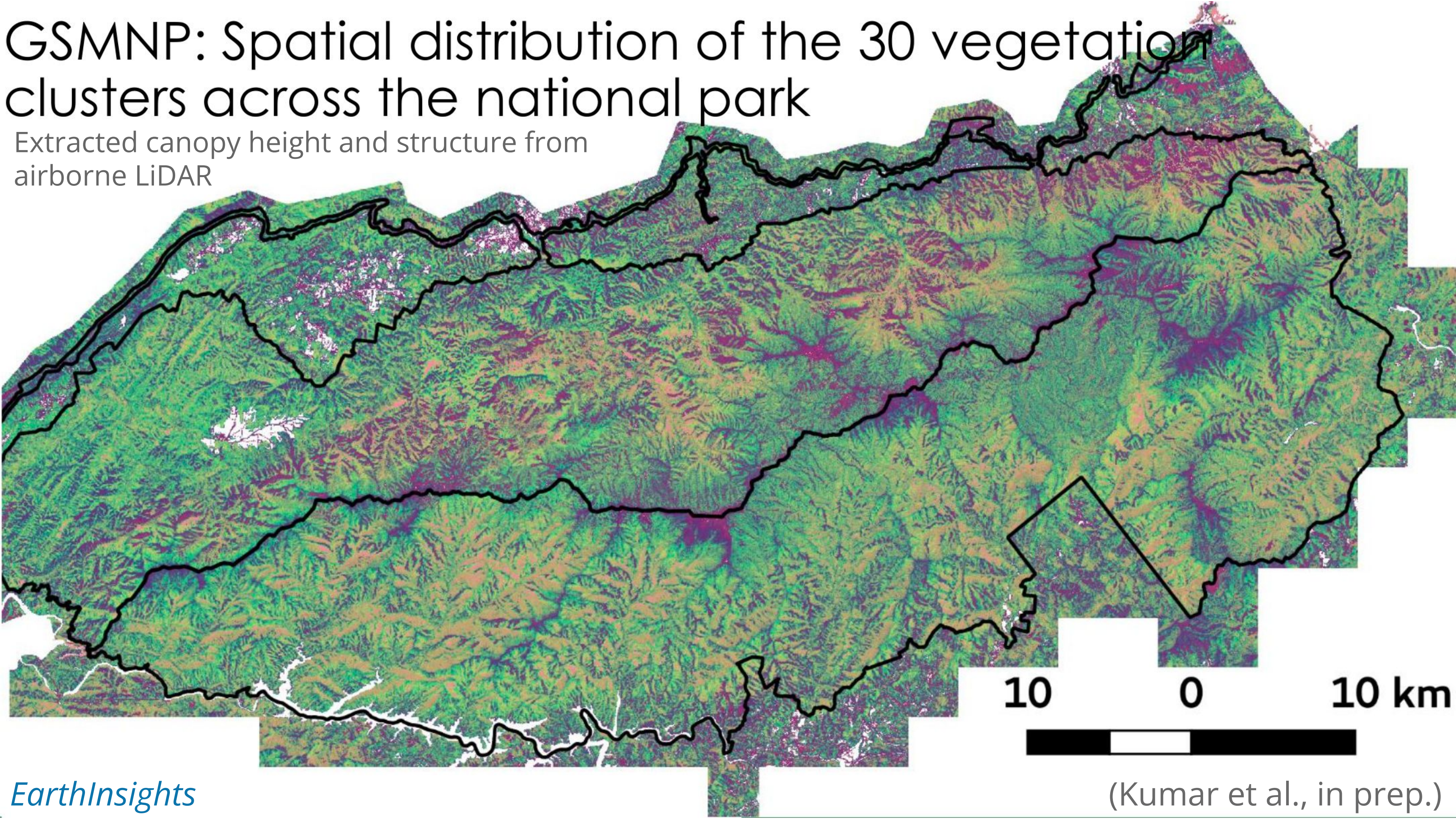
PC1 ~ Evergreen
PC2 ~ Deciduous
PC3 ~ Dry Deciduous

EarthInsights

(Hargrove et al., in prep.)

GSMNP: Spatial distribution of the 30 vegetation clusters across the national park

Extracted canopy height and structure from airborne LiDAR



EarthInsights

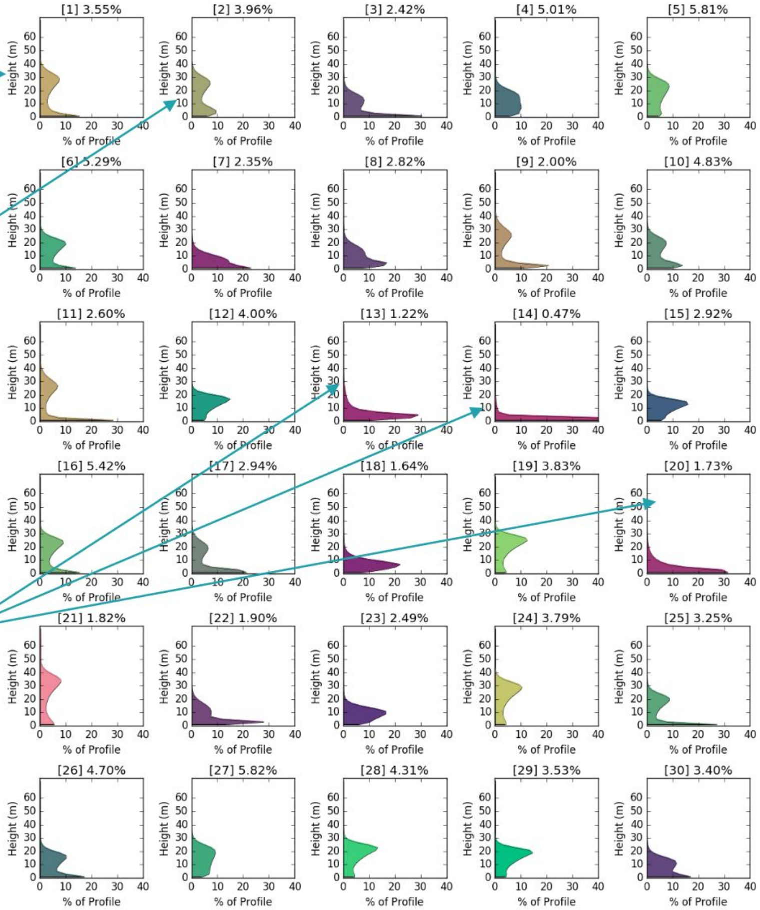
(Kumar et al., in prep.)

GSMNP: 30 representative vertical structures (cluster centroids) identified

tall forests with low understory vegetation

forests with slightly lower mean height with dense understory vegetation

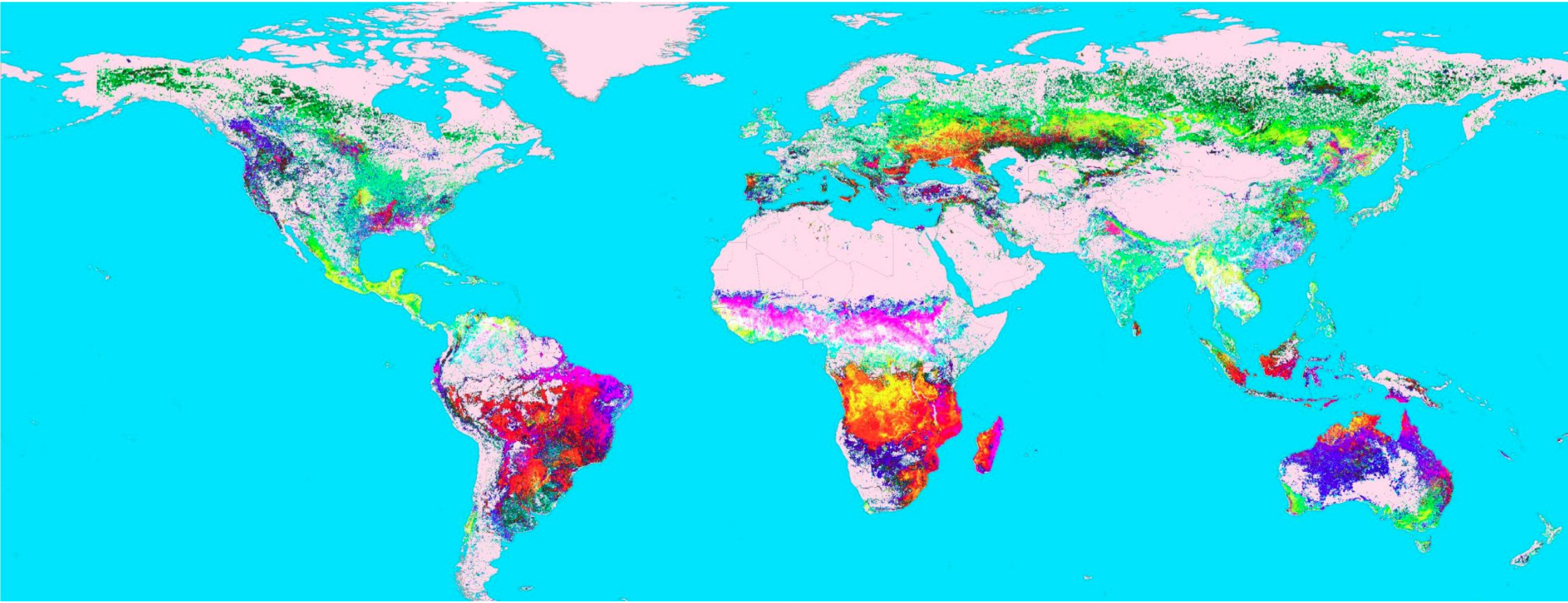
low height grasslands and heath balds that are small in area but distinct landscape type



EarthInsights

(Kumar et al., in prep.)

Global Fire Regimes

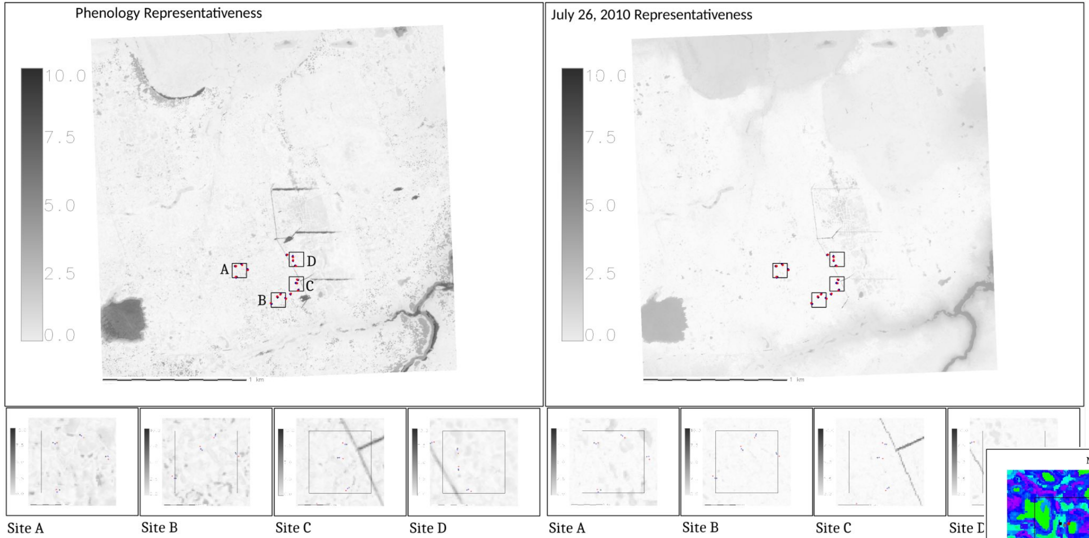


Regions that exhibit similar fire seasonality globally

From MODIS “Hotspots” at 1 km resolution from 2002–2018

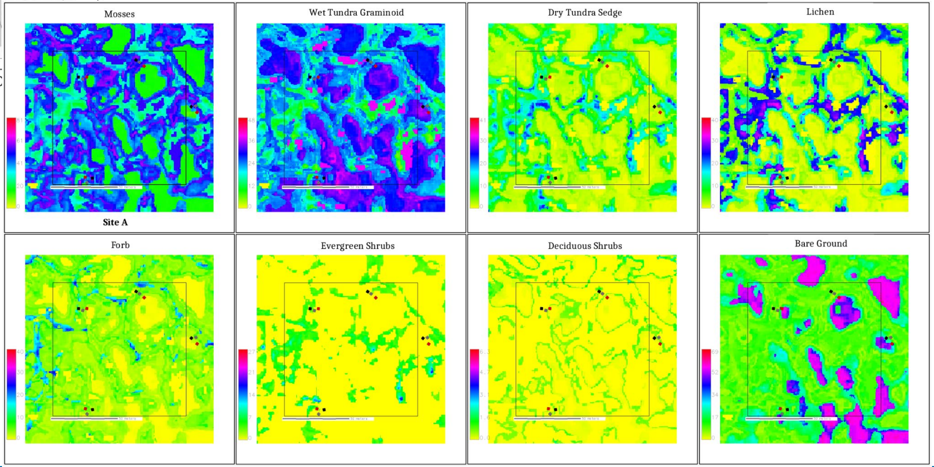
(Norman et al., submitted)

Vegetation Distribution at Barrow Environmental Observatory



Representativeness map for vegetation sampling points in sites A, B, C, and D with phenology (left) and without (right) from WorldView2 multispectral imagery for the year 2010 and LiDAR data

Example plant functional type (PFT) distributions scaled up from vegetation sampling locations

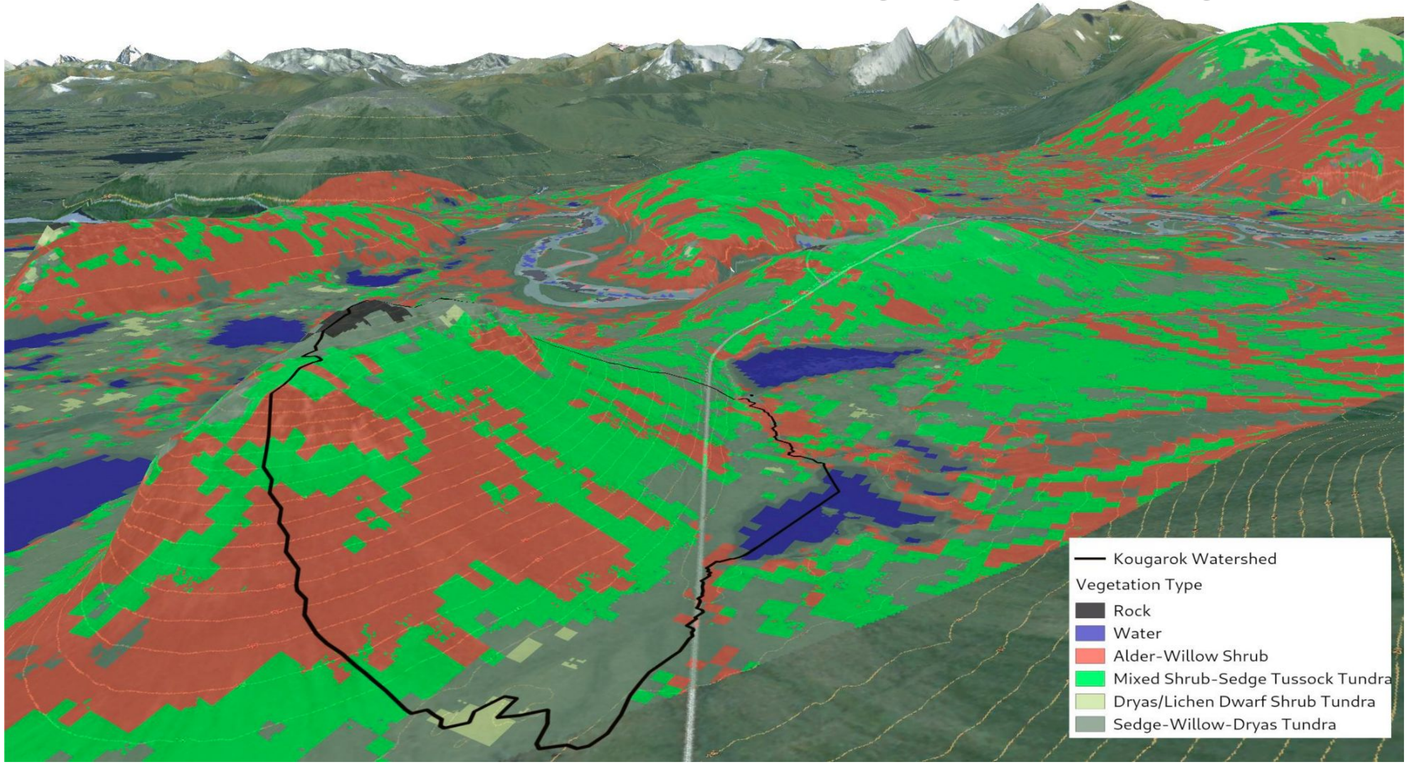


In situ data from field measurement activities inform the development of wide-scale maps of vegetation distribution through inference using remote sensing data as surrogate variables, and relationships with environmental controls can be extracted

Langford, Z. L., et al. (2016), Mapping Arctic Plant Functional Type Distributions in the Barrow Environmental Observatory Using WorldView-2 and LiDAR Datasets, *Remote Sens.*, 8(9):733, doi:10.3390/rs8090733.

Arctic Vegetation Mapping from Multi-Sensor Fusion

Used Hyperion Multispectral and IfSAR-derived Digital Elevation Model, applied cluster analysis, and trained a convolutional neural network (CNN) with Alaska Existing Vegetation Ecoregions (AKEVT)



Langford, Z. L., et al. (2019), Arctic Vegetation Mapping Using Unsupervised Training Datasets and Convolutional Neural Networks, *Remote Sens.*, 11(1):69, doi:[10.3390/rs11010069](https://doi.org/10.3390/rs11010069).

Satellite Data Analytics Enables Within-Season Crop Identification

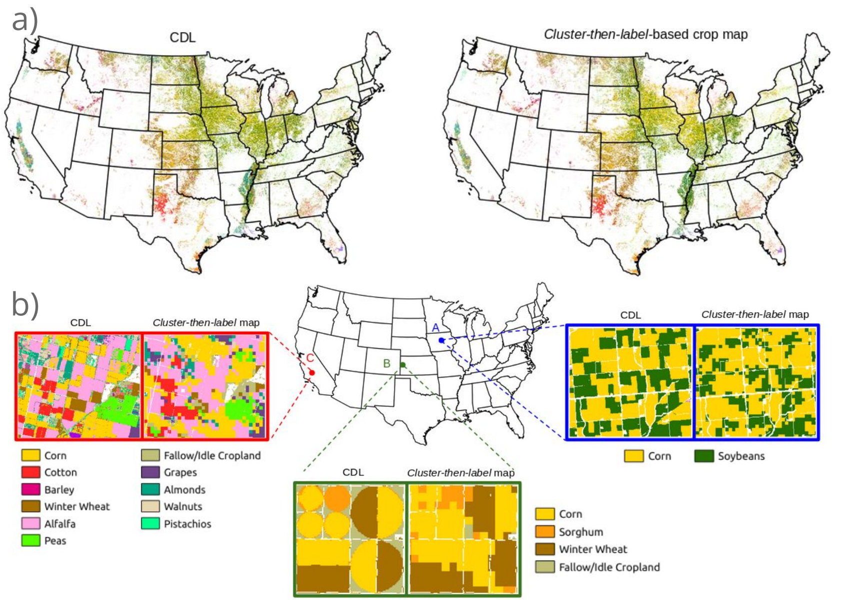
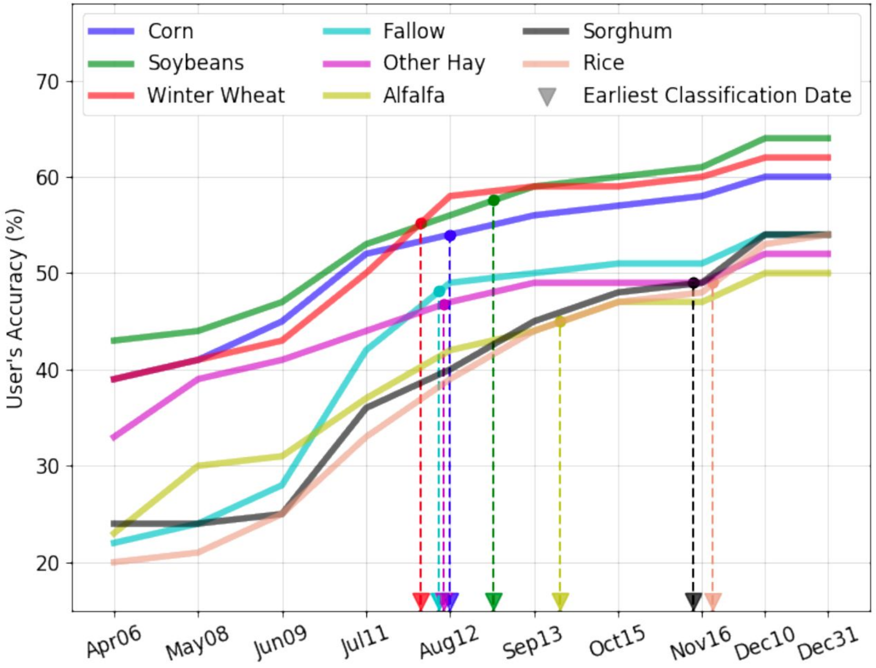


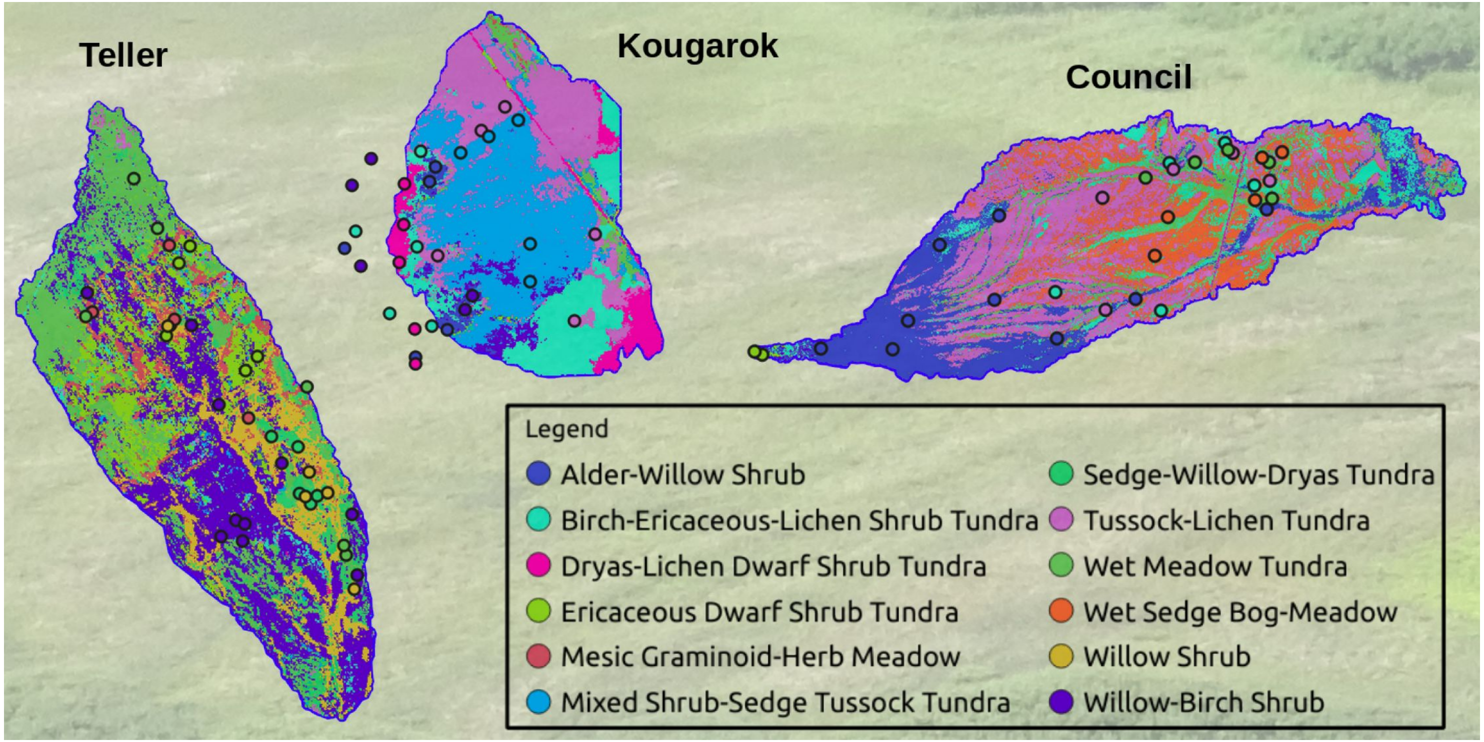
Figure: a) Comparison of cluster-then-label crop map with USDA Crop Data Layer (CDL) shows similar patterns at continental scale. b) Good spatial agreement is found at three selected regions, but cluster-then-label crop maps lack sharpness at field boundaries due to coarser resolution of MODIS data.

Earliest date for crop type classification



Konduri, V. S., J. Kumar, W. W. Hargrove, F. M. Hoffman, and A. R. Ganguly (2020), Mapping Crops Within the Growing Season Across the United States, *Remote Sens. Environ.*, 251, 112048, doi:10.1016/j.rse.2020.112048.

Watershed-Scale Plant Communities Determined from DNN and AVIRIS-NG



At the watershed scale, vegetation community distribution follows topographic and water controls. At a fine scale, nutrients limit the distribution of vegetation types.

(Konduri et al., in prep.)

Leveraging Advances in Machine Learning for Earth Sciences

Existing and new domain-specific machine learning techniques can improve understanding of biospheric processes and representation in Earth system models

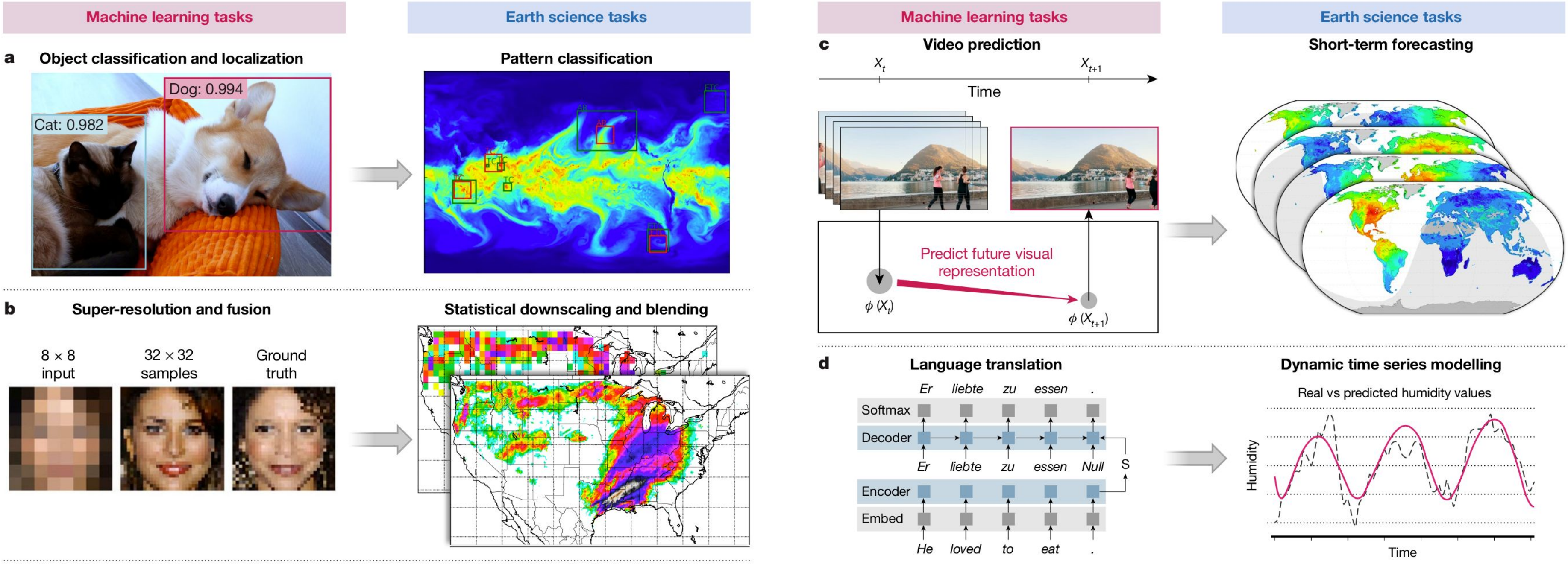
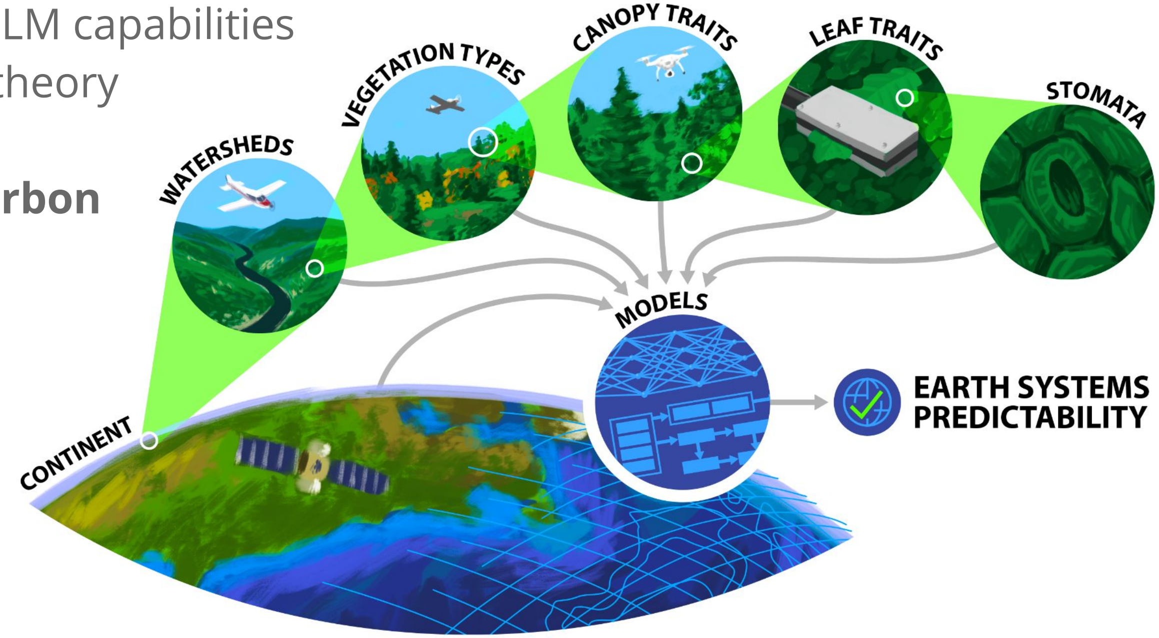


Figure 2 in Reichstein et al. (2019)

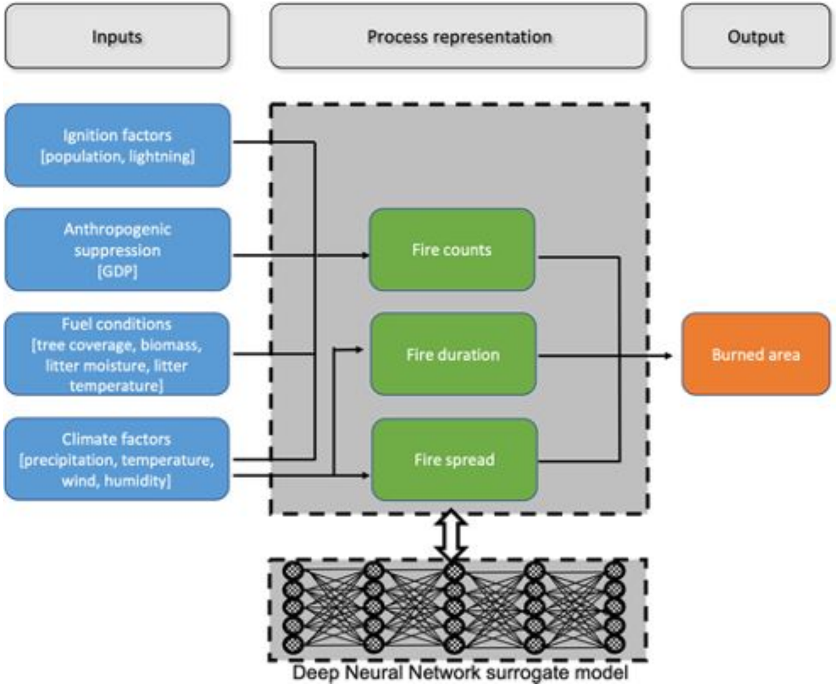
Machine Learning for Understanding Biospheric Processes

- Widening adoption of deep neural networks and growth of climate data are fueling interest in AI/ML for use in weather and climate and Earth system models
- ML potential is high for improving predictability when (1) *sufficient data are available for process representations* and (2) *process representations are computationally expensive*
- Example methods for improving ELM capabilities by exploring ML and information theory approaches:
    - **Soil organic carbon & radiocarbon**
    - **Wildfire**
    - **Methane emissions**
    - **Ecohydrology**
- All of these applications involve unresolved, subgrid-scale processes that strongly influence results at the largest scales



Hybrid Modeling of Wildfire Activities

- Improve model simulations of **wildfire processes**, including ignition, fire duration, and spread rate with Deep Neural Network models
- Improve simulated **wildfire emissions** and their impacts on atmospheric properties, including aerosols, greenhouse gases, phosphorus transport, and pollutants
- Improve the projection of near-future and long-term dynamics of wildfire activities
- Accelerate E3SM coupled land–atmosphere modeling activities for wildfire research
- Explore online ML training/validation strategy for E3SM coupled model simulations

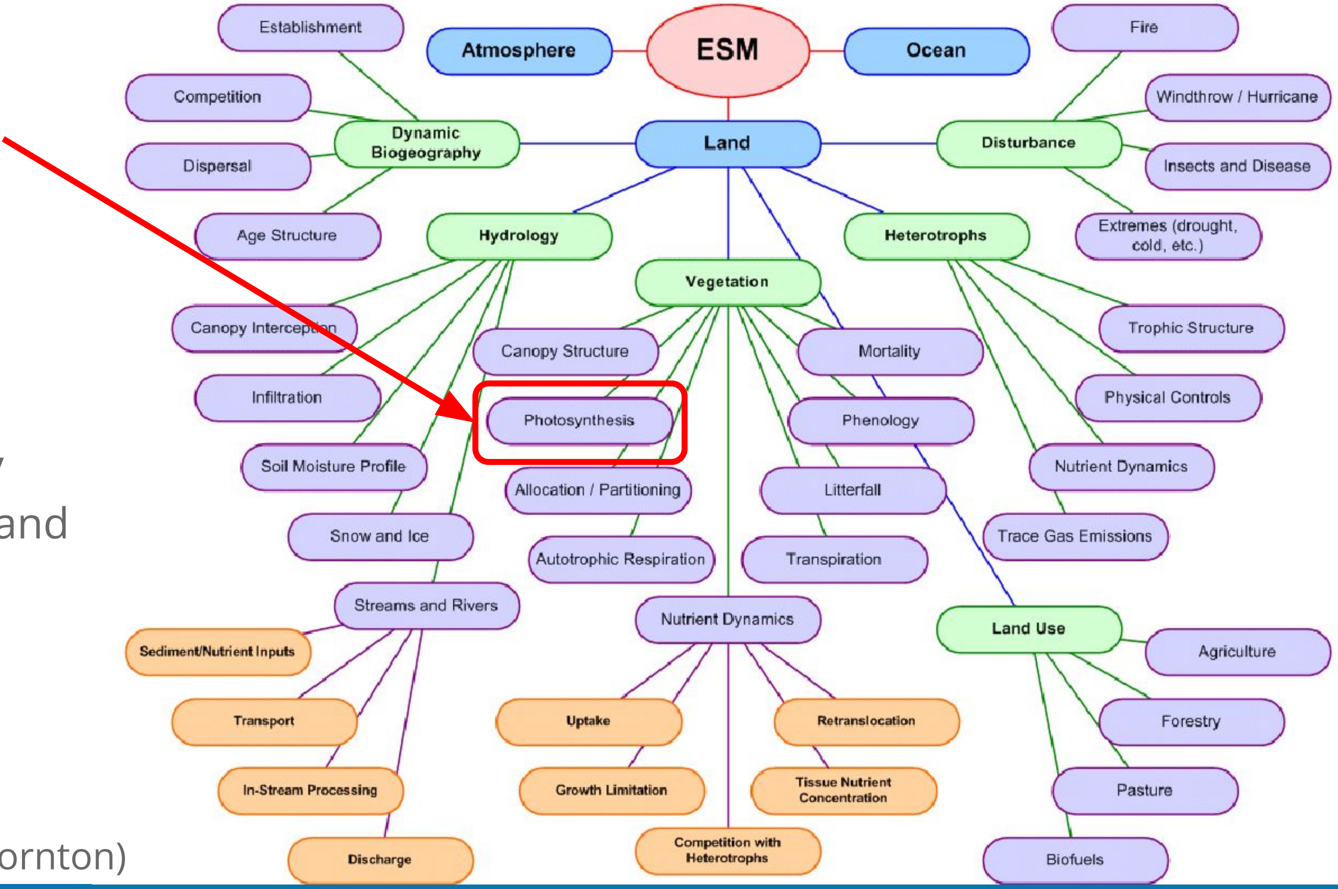


Zhu et al. (2022)

Hybrid ML/Process-based Modeling for Terrestrial Modeling

In the hierarchy of land model processes, we start with the **photosynthesis** parameterization because

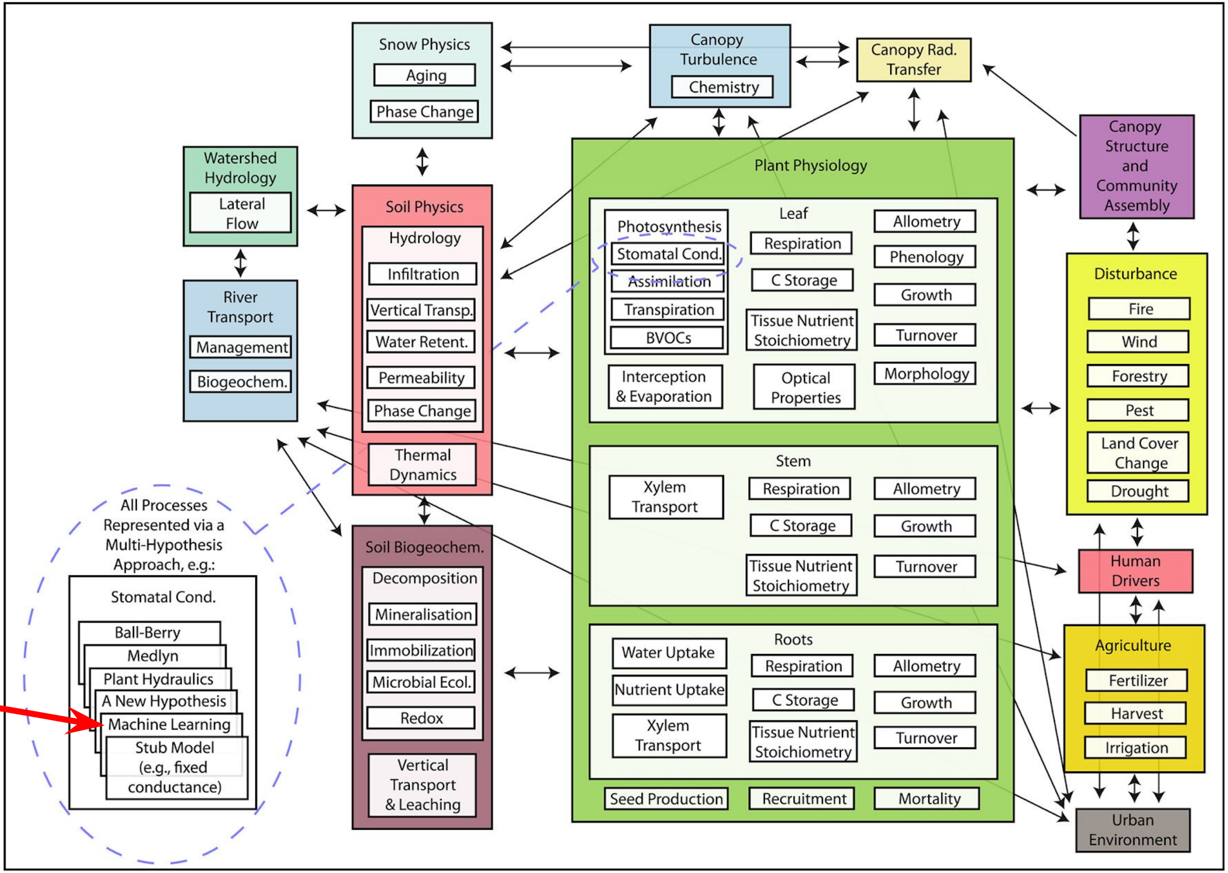
- Multiple hypotheses
- Many leaf-level measurements
- Most computationally intensive part of the land model



(Figure from P. E. Thornton)

Hybrid ML/Process-based Modeling for Terrestrial Modeling

Individual processes can be represented in a multi-hypothesis approach, and ML provides an opportunities for (1) a model surrogate module or (2) a data-derived module that can be further explored or used to calibrate other hypotheses, when sufficient data are available.



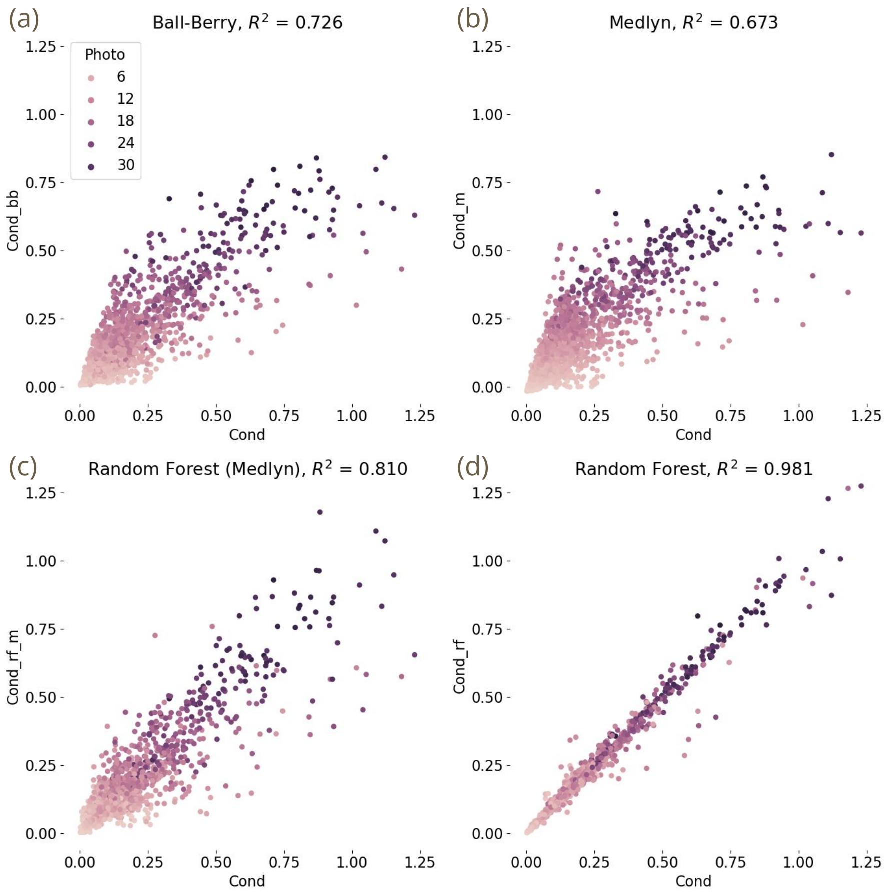
(a) Process Schematic of a Possible Full-Complexity Configuration of a Land Surface Model

(Fisher and Koven, 2020)

Hybrid Modeling of Photosynthesis and Ecohydrology

- Significant leaf-level data may be used to train ML parameterizations to **improve accuracy** and **computational performance**
- **Estimated stomatal conductance** vs. measured stomatal conductance for (a) Ball-Berry, (b) Medlyn, (c) Random forest (with Medlyn inputs), and (d) Random forest with all inputs from Lin et al. (2015)
- Inputs to the Medlyn parameterization are leaf-level CO_2, photosynthesis, and vapor pressure deficit
- Random forest trained on these three inputs (c) performs slightly better than Medlyn
- Random forest trained on more variables (d) achieves an R^2 of 0.98

(Massoud, Collier, et al. in prep)

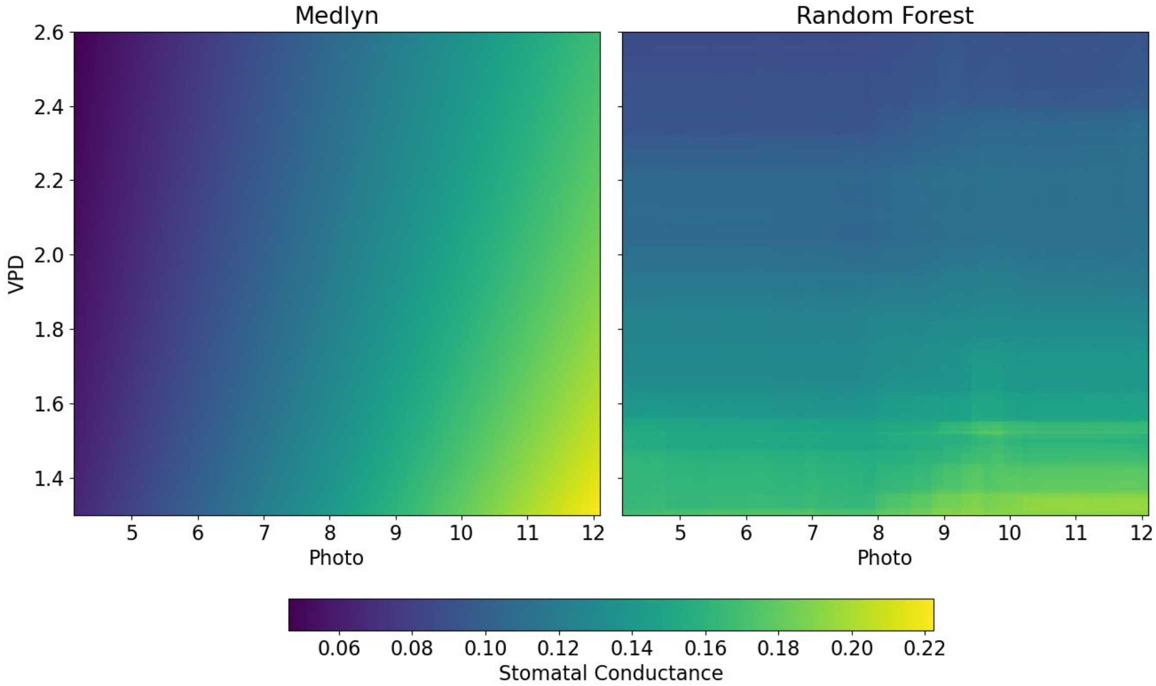


Hybrid Modeling of Photosynthesis and Ecohydrology

- Most process-based or empirical formulations are continuous
- But ML formulations may exhibit discontinuities in the multi-dimensional space of inputs because of out-of-sample data or artifacts of sampling or precision

- For example, we can see such discontinuities at right for Random Forest in the VPD vs. photosynthesis heat map for stomatal conductance

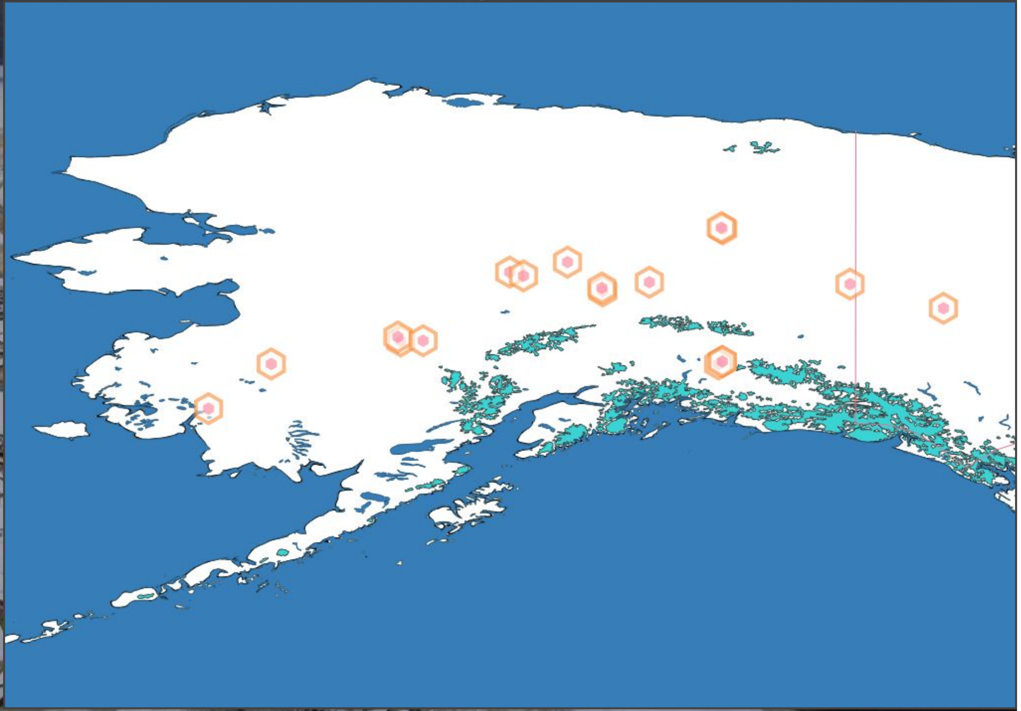
- These discontinuities are likely to have numerical consequences when attempting to couple a ML parameterization into a hybrid empirical / ML Earth system model



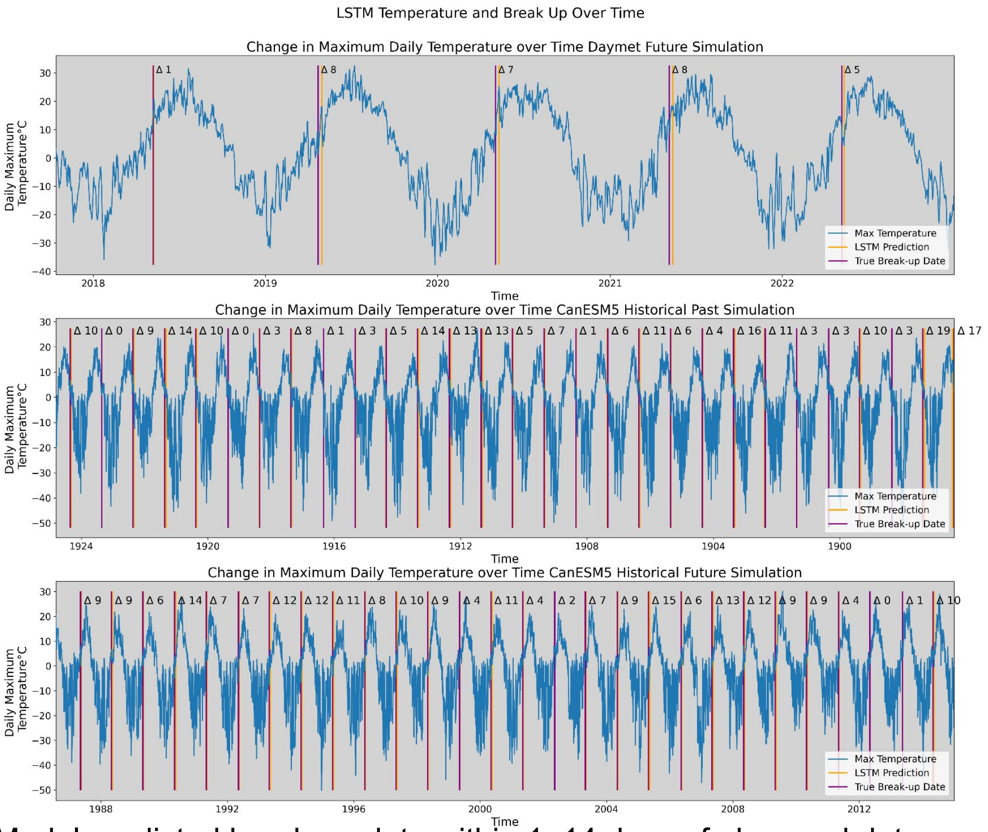
(Massoud, Collier, et al. in prep)

orecasting River Ice Breakup using Machine Learning

- Study sites were selected at long term river ice monitoring stations in Yukon river basin.
- We developed Long Short Term Memory (LSTM) and transformer models to predict river ice breakups.
- Primary predictor variables: daily min/max air temp., precipitation, snow water eq., shortwave radiation
- Datasets: DAYMET, CanESM5 (Historical, SSP119, SSP370, SSP585, SSP534-over)

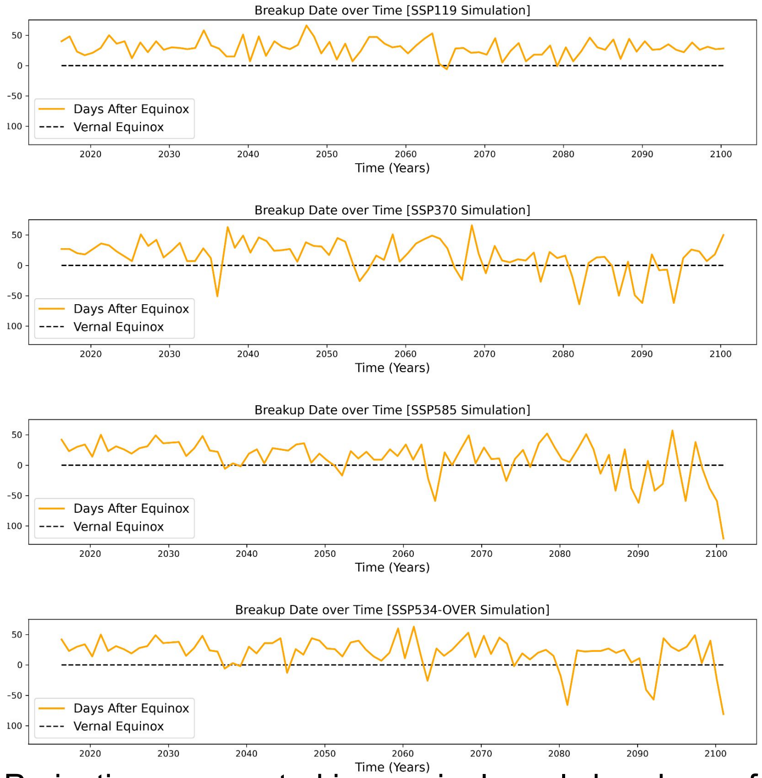


Break-up date predictions for historical period



Model predicted break-up date within 1–14 days of observed dates.

Break-up date predictions under future scenarios



Projections suggested increasingly early break-up of river ice under warming scenarios.

(Limber et al., 2025)

AI4ESP

ARTIFICIAL INTELLIGENCE FOR EARTH SYSTEM PREDICTABILITY (AI4ESP): CHALLENGES AND OPPORTUNITIES

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SCOTT M. COLLIS
Argonne National Laboratory

U.S. DEPARTMENT OF ENERGY

https://ai4esp.org/ https://ai4esp.slack.com/

AI4ESP | Artificial Intelligence for Earth System Predictability

A multi-lab initiative working with the Earth and Environmental Systems Science Division (EESSD) of the Office of Biological and Environmental Research (BER) to develop a new paradigm for Earth system predictability focused on enabling artificial intelligence across field, lab, modeling, and analysis activities.

White papers were solicited for development and application of AI methods in areas relevant to EESSD research with an emphasis on quantifying and improving Earth system predictability, particularly related to the integrative water cycle and extreme events.

How can DOE directly leverage artificial intelligence (AI) to engineer a substantial (paradigm-changing) improvement in Earth System Predictability?

156 white papers were received and read to plan the organization of the **AI4ESP Workshop on Oct 25–Dec 3, 2021**

U.S. DEPARTMENT OF ENERGY

Earth System Predictability Sessions

- Atmospheric Modeling
- Land Modeling
- Human Systems & Dynamics
- Hydrology
- Watershed Science
- Ecohydrology
- Aerosols & Clouds
- Climate Variability & Extremes
- Coastal Dynamics, Oceans & Ice

Cross-Cut Sessions

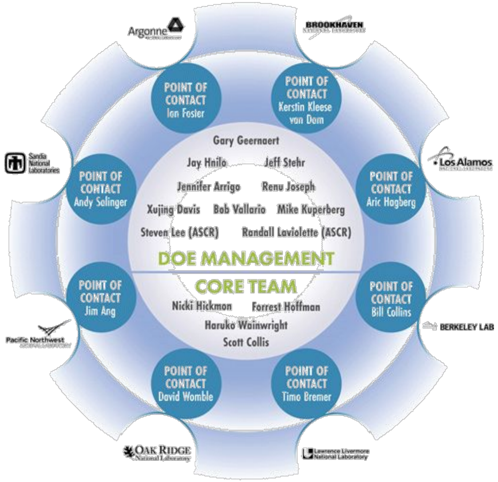
- Data Acquisition
- Neural Networks
- Surrogate models and emulators
- Knowledge-Informed Machine Learning
- Hybrid Modeling
- Explainable/Interpretable/Trustworthy AI
- Knowledge Discovery & Statistical Learning
- AI Architectures and Co-design

Workshop Report

- Posted on ai4esp.org
- Executive Summary
- Long summary
- Earth science chapters
- Computational science chapters

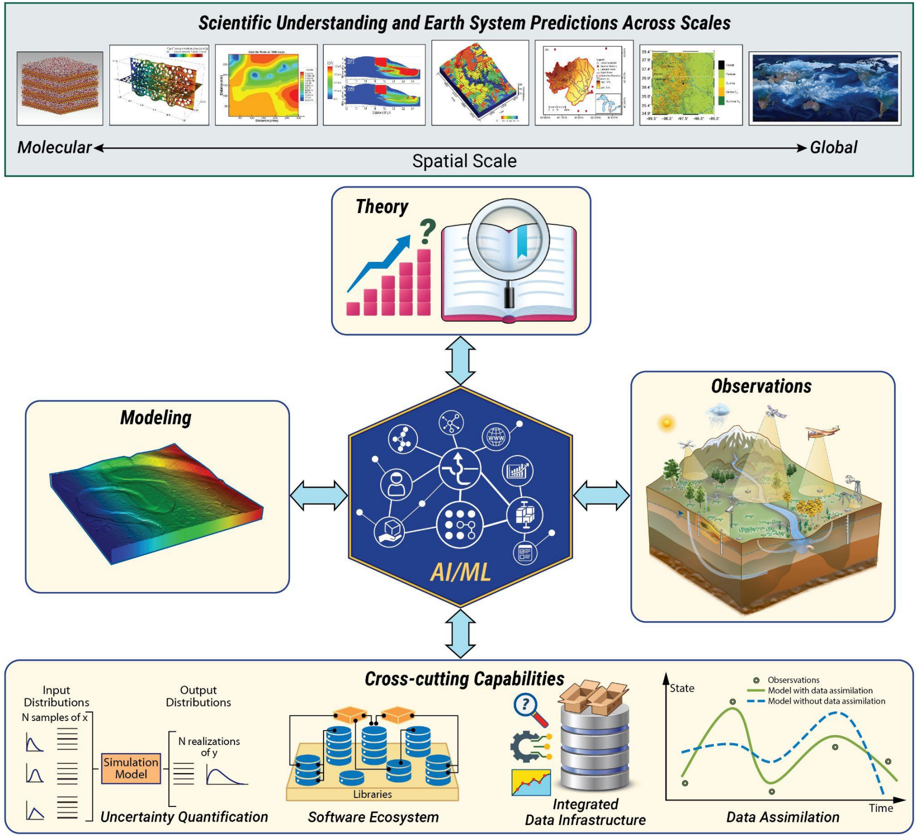
AMS Special Collection

- In thenew AI for the Earth Systems journal



AI4ESP

AI4ESP WORKSHOP HIGHLIGHTS



EESA22-032

U.S. DEPARTMENT OF ENERGY

AI4ESP

AI4ESP WORKSHOP HIGHLIGHTS

Overview of priorities emerging from the AI4ESP workshop across 3 key themes.

These priorities will help address major challenges for Earth system predictability

Earth Science Priorities

- New observations
- AI-ready data products
- Data-driven and hybrid models
- Analytical approaches
- Uncertainty quantification, model parametrization & calibration

To Tackle Challenges

- Significant data gaps
- Scaling and heterogeneity
- Extreme events
- Representation of human activities
- Knowledge discovery
- Accurate high-resolution predictions with low bias, uncertainty
- Providing actionable, timely information for decision making

Computational Science Priorities

- Hybrid models
- Fundamental math and algorithms
- Interpretable, trustworthy AI
- AI-enabled data acquisition
- Data, software, hardware infrastructure

To Tackle Challenges

- Physically consistent predictions for data-driven models
- Computational costs of process models
- Sparse data, extreme values
- Identifying causality
- Interpretable, trustworthy predictions
- Data discovery, access, synthesis
- Model development and comparison

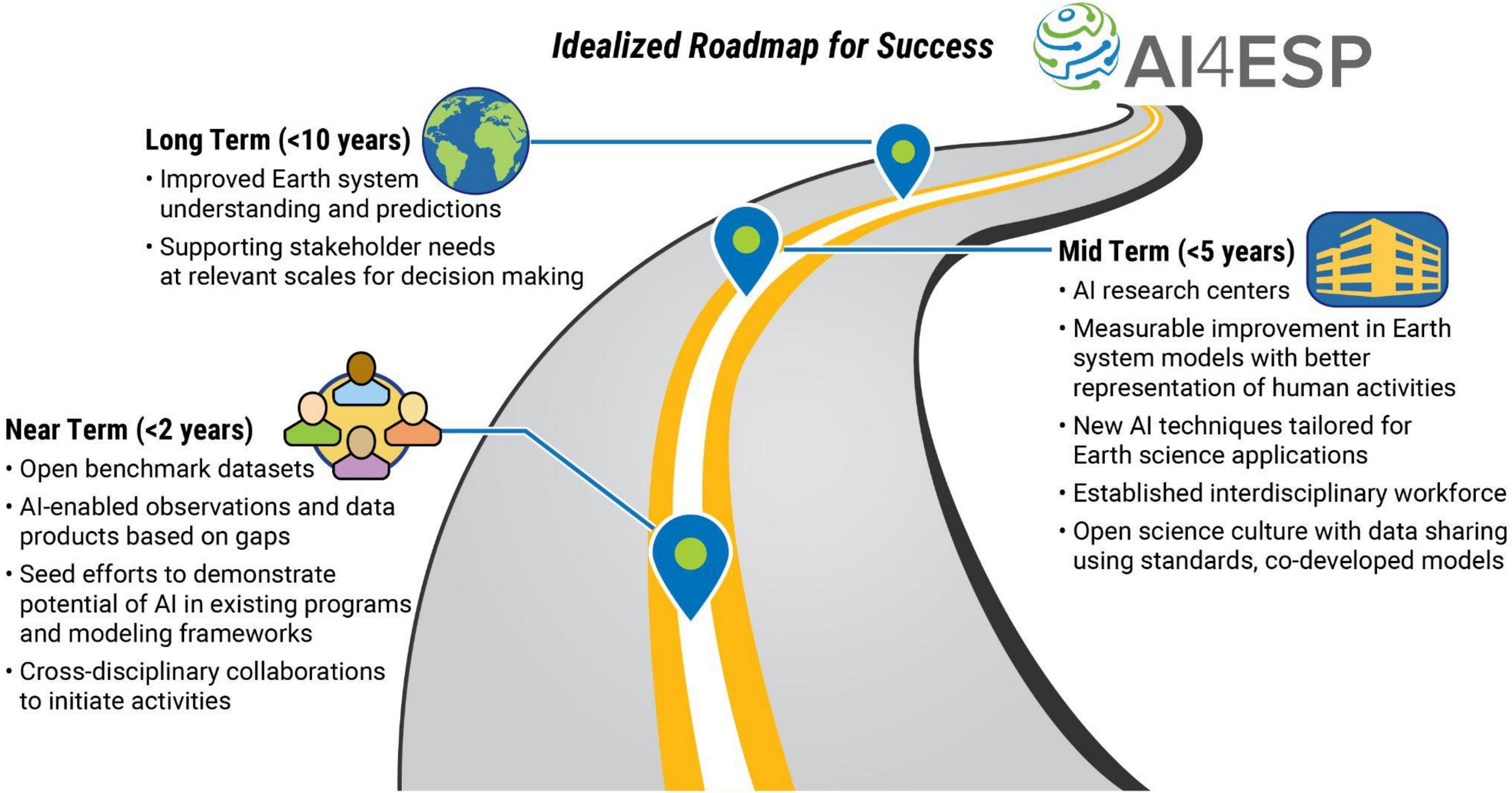
Programmatic and Cultural Priorities

- AI research centers
- Workforce development
- Codesign infrastructure
- Common standards, benchmarks
- Seed projects, integrate AI into programs
- AI ethics and policies

To Tackle Challenges

- Interdisciplinary scientific research
- Diverse organizational missions
- Personnel lack training in AI/ML
- Using data, communicating across research domains, organizations
- Data bias, model fairness, explainability of predictions

AI4ESP WORKSHOP HIGHLIGHTS



Reducing Uncertainties in Biogeochemical Interactions through Synthesis and Computation (RUBISCO)

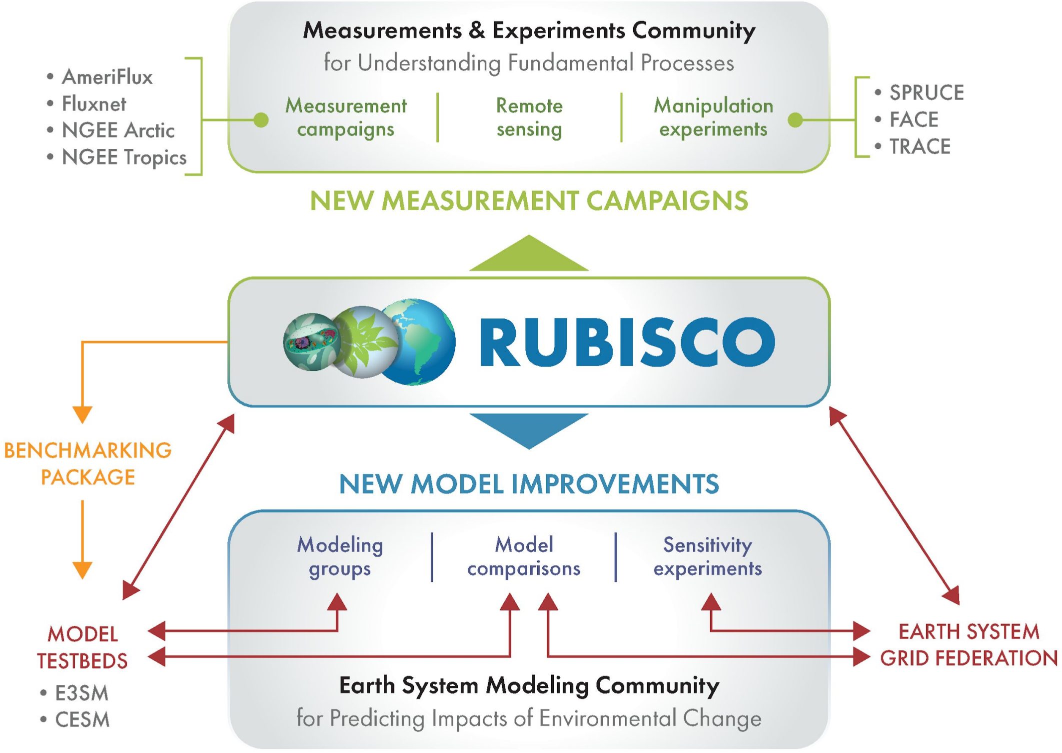
EESM-RGMA RUBISCO Science Focus Area (SFA)

Forrest M. Hoffman (Laboratory Research Manager), Charles D. Koven (Science Co-Lead), and James T. Randerson (Chief Scientist)

RUBISCO Research Goals

- Identify and quantify interactions between biogeochemical cycles and the Earth system
- Quantify and reconcile uncertainties in Earth system models (ESMs) associated with those interactions

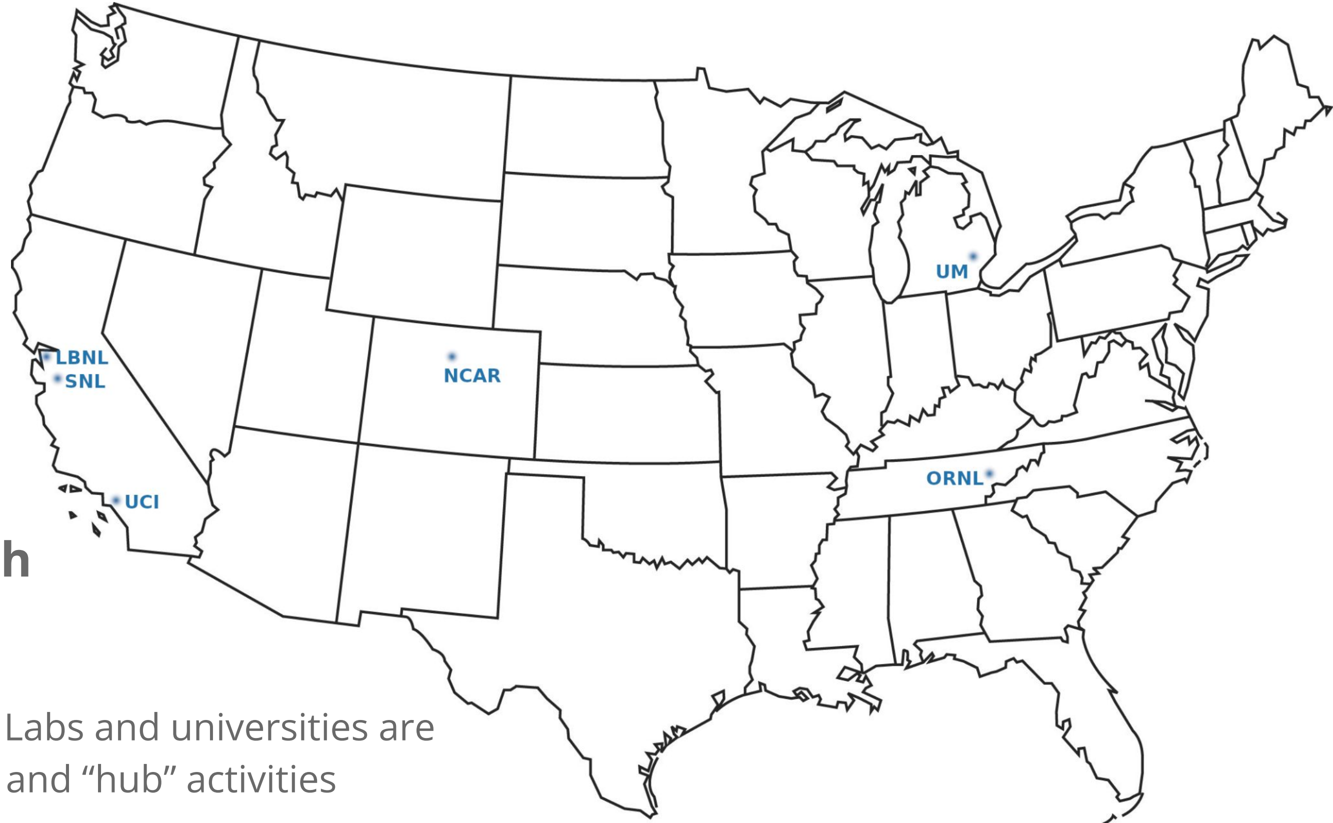
The RUBISCO SFA works with the measurements and the modeling communities to use best-available data to evaluate the fidelity of ESMs. RUBISCO identifies model gaps and weaknesses, informs new model development efforts, and suggests new measurements and field campaigns.



Berkeley Lab · NCAR National Center for Atmospheric Research · Oak Ridge National Laboratory · Sandia National Laboratories · The University of California Irvine · Michigan

RUBISCO Consists of Six Partner Institutions

- **3 DOE National Labs**
  - Lawrence Berkeley (LBNL)
  - Oak Ridge (ORNL)
  - Sandia (SNL)
- **2 Universities**
  - U. California Irvine (UCI)
  - U. Michigan (UM)
- **National Center for Atmospheric Research (NCAR)**



Collaborations at other National Labs and universities are fostered by our Working Groups and “hub” activities

RUBISCO Phase 3 Research & Development Objectives

1. Pursue **hypothesis-driven research** to quantify uncertainties related to estimates of contemporary terrestrial and ocean processes
2. Apply new advances in the field of **artificial intelligence (AI) and machine learning (ML)** to improve prediction and simulation of biospheric processes
3. Assess the impact of **biogeochemical interactions** on Earth system variability
4. Explore **ecological & hydrological interactions** through simulation, analysis, & benchmarking using the Energy Exascale Earth System Model (E3SM) & CESM
5. Develop & apply our open source **ILAMB and IOMB benchmarking software** tools for evaluation of ESM biogeochemical & hydrological processes
6. Manage **Working Groups** that engage community researchers and RUBISCO scientists in data synthesis, multi-model analysis, and benchmarking
7. Conduct **ensemble and parameter simulations** to explore interactions

Science Questions Span Temporal and Spatial Scales

Science Questions

1. How can observational constraints and models be used to identify and quantify uncertainties in terrestrial and oceanic processes?
2. How can advances in machine learning be leveraged to improve understanding of biospheric processes and their representation in Earth system models?
3. What is the contribution of biogeochemical interactions to future Earth system variability on seasonal, interannual, and decadal timescales?
4. What are the key pathways and strengths of multiscale ecological and hydrological interactions?

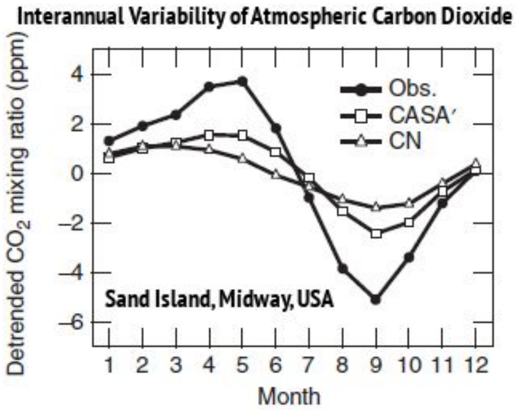
Community Resource Objectives

1. Advance ILAMB & IOMB
2. Manage SOM, AmeriFlux, and Soil Moisture Working Groups
3. Biogeochemical-water cycle simulations

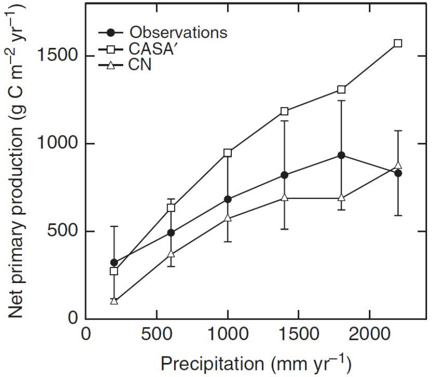
International Land Model Benchmarking (ILAMB)

What is a Benchmark?

- A **benchmark** is a quantitative test of model function achieved through comparison of model results with observational data
- Acceptable performance on a benchmark **is a necessary but not sufficient condition** for a fully functioning model
- **Functional relationship benchmarks** offer tests of model responses to forcings and yield insights into ecosystem processes
- Effective benchmarks must draw upon **a broad set of independent observations** to evaluate model performance at multiple scales



Models often fail to capture the amplitude of the seasonal cycle of atmospheric CO_2



Models may reproduce correct responses over only a limited range of forcing variables

(Randerson et al., 2009)

Why Benchmark Models?

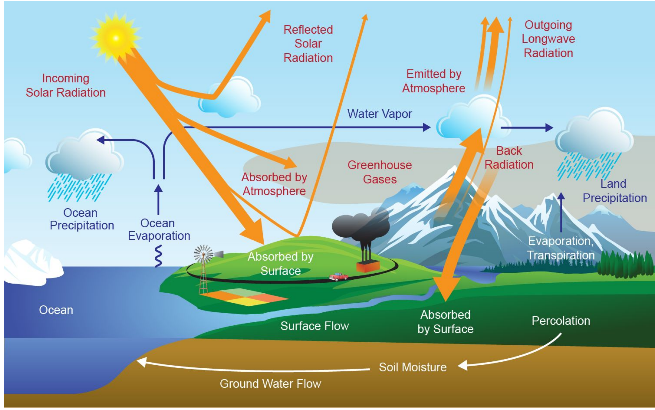
- To **quantify and reduce uncertainties** in carbon cycle feedbacks to improve projections of future climate change (Eyring et al., 2019; Collier et al., 2018)
- To **diagnose impacts of process-based or machine learning model development** on process representations and their interactions
- To **guide synthesis efforts**, such as the Intergovernmental Panel on Climate Change (IPCC), by determining which models are broadly consistent with observations (Eyring et al., 2019)
- To **increase scrutiny of key datasets** used for model evaluation
- To **identify gaps in existing observations** needed to inform model development
- To **accelerate delivery of new measurement datasets** for rapid and widespread use in model assessment

What is ILAMB?

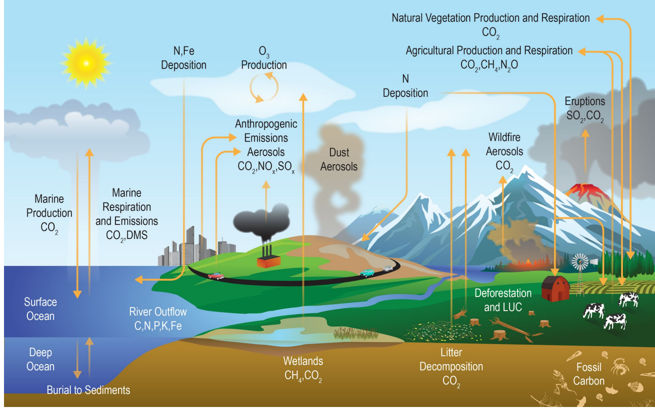
RUBISCO

A community coordination activity created to:

- **Develop internationally accepted benchmarks** for land model performance by drawing upon collaborative expertise
- **Promote the use of these benchmarks** for model intercomparison
- **Strengthen linkages between experimental, remote sensing, and Earth system modeling communities** in the design of new model tests and new measurement programs
- **Support the design and development of open source benchmarking tools**



Energy and Water Cycles

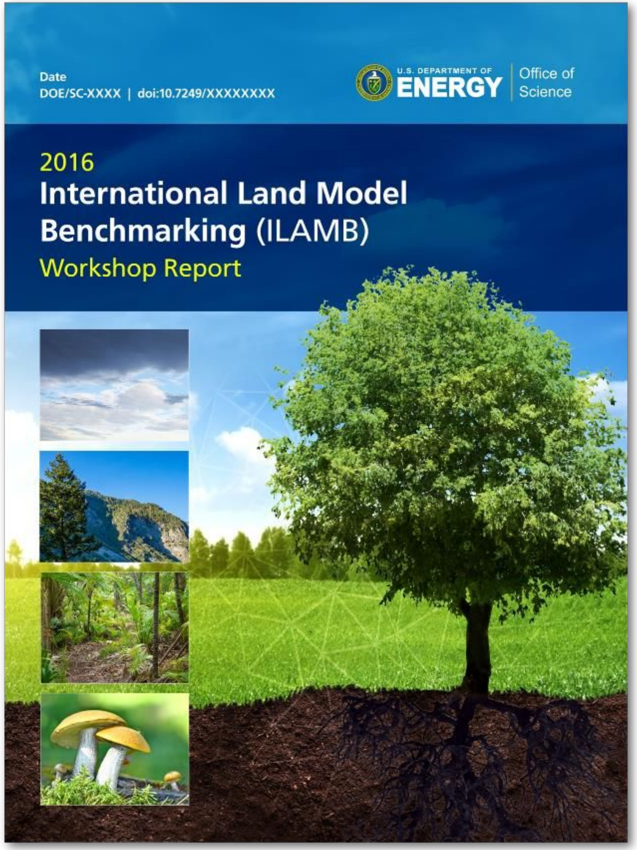


Carbon and Biogeochemical Cycles

Berkeley Lab
NCAR National Center for Atmospheric Research
Oak Ridge National Laboratory
Sandia National Laboratories
Michigan

- **First ILAMB Workshop** was held in Exeter, UK, on June 22–24, 2009
- **Second ILAMB Workshop** was held in Irvine, CA, USA, on January 24–26, 2011
  - ~45 researchers participated from the US, Canada, UK, Netherlands, France, Germany, Switzerland, China, Japan, and Australia
  - Developed methodology for model-data comparison and baseline standard for performance of land model process representations (Luo et al., 2012)

2016 International Land Model Benchmarking (ILAMB) Workshop
May 16–18, 2016, Washington, DC



(Hoffman et al., 2017)

Third ILAMB Workshop was held May 16–18, 2016

- Workshop Goals
  - Design of new metrics for model benchmarking
  - Model Intercomparison Project (MIP) evaluation needs
  - Model development, testbeds, and workflow processes
  - Observational datasets and needed measurements
- Workshop Attendance
  - 60+ participants from Australia, Japan, China, Germany, Sweden, Netherlands, UK, and US (10 modeling centers)
  - ~25 remote attendees at any time

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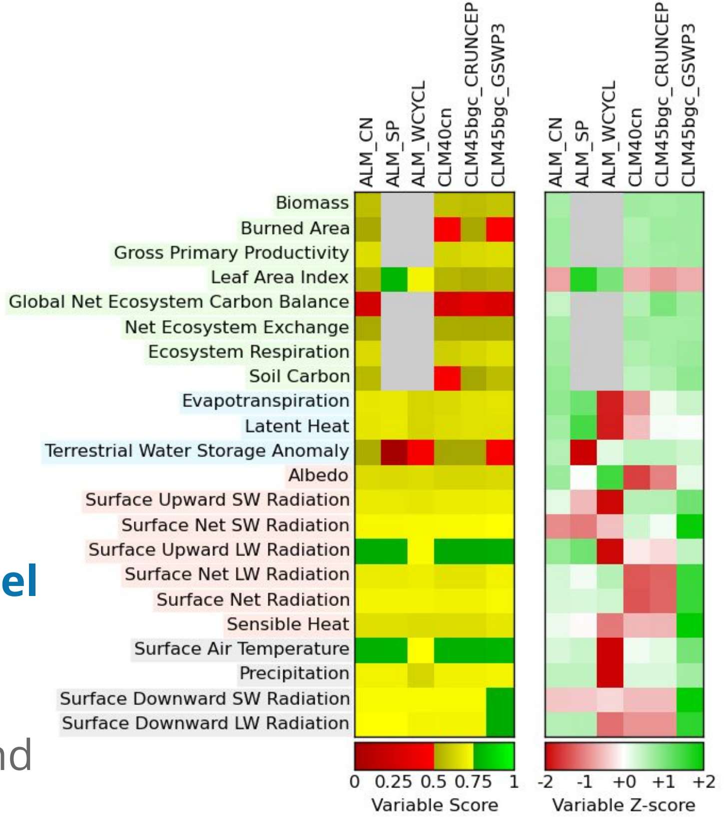
2025 ILAMB Meeting in New Orleans (December 2025)

60+ participants from 6 countries — Report coming soon!

Development of ILAMB Packages

- **ILAMBv1** released at 2015 AGU Fall Meeting Town Hall, doi:[10.18139/ILAMB.v001.00/1251597](https://doi.org/10.18139/ILAMB.v001.00/1251597)
- **ILAMBv2** released at 2016 ILAMB Workshop, doi:[10.18139/ILAMB.v002.00/1251621](https://doi.org/10.18139/ILAMB.v002.00/1251621)
- **ILAMBv3** released at 2025 ILAMB Meeting
- **Open Source software** written in Python; **runs in parallel** on laptops, clusters, and supercomputers
- Routinely used for land model evaluation during development of ESMs, including the **E3SM Land Model** (Zhu et al., 2019) and the **CESM Community Land Model** (Lawrence et al., 2019)
- Used to evaluate **TRENDY models** for annual GCB
- **Models are scored** based on statistical comparisons and functional response metrics



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Dashboard Refresh

EcosystemandCarbonCycle | GlobalNetEcosystemCarbonBalance | Hoffman-1-0

MODEL
CanESM5

REGION
Global - Land

MODE
Single Model (All Plots)
All Models (By Plot)

ANALYSIS TYPES
All
nbp

DATA INFORMATION

Title
Land anthropogenic carbon flux estimates

Institution
University of California at Irvine, Irvine, CA, USA; Oak Ridge National Laboratory, Oak Ridge, TN, USA

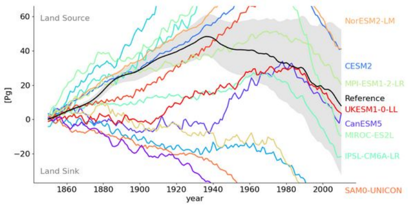
Version
v20251117

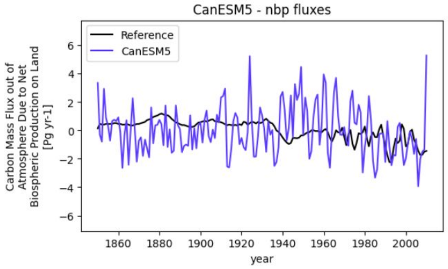
Doi
N/A

Scalar Table

source	nbp(2010) [Pg]	diff(2010) [Pg]	Difference Score [1]	Trajectory Score [1]	Overall Score [1]
ACCESS-ESM1-5	-0.28	1.17	0.99	0.07	0.53
CanESM5	5.27	6.72	0.93	0.06	0.49
CESM2	0.28	1.73	0.98	0.11	0.54
CMCC-ESM2	-1.28	0.17	1.00	0.07	0.53
EC-Earth3-Veg	-0.98	0.47	0.99	0.06	0.53
GFDL-ESM4	0.46	1.91	0.98	0.05	0.51
IPSL-CM6A-LR	0.34	1.79	0.98	0.09	0.53
MIROC-ES2L	-0.45	1.00	0.99	0.05	0.52
MPI-ESM1-2-LR	-1.95	-0.50	0.99	0.08	0.54
MRI-ESM2-0	-0.15	1.30	0.99	0.06	0.52
NorESM2-LM	-0.10	1.35	0.98	0.10	0.54
Reference	-1.45				
SAM0-UNICON	2.24	3.69	0.96	0.08	0.52
TaiESM1	1.39	2.84	0.97	0.07	0.52
UKESM1-0-LL	-0.74	0.71	0.99	0.07	0.53

nbp





Show results by model or by plot

Analysis type can be clicked to reduce table and number of plots

Reference data details

Click to sort by any column

Colors highlight what is below (orange) or above (purple) the selected row

ILAMB Produces Diagnostics and Scores Models

- ILAMB generates a top-level **portrait plot** of models scores
- For every variable and dataset, ILAMB can automatically produce
  - **Tables** containing individual metrics and metric scores (when relevant to the data), including
    - Benchmark and model **period mean**
    - **Bias** and **bias score** (S_{bias})
    - **Root-mean-square error (RMSE)** and **RMSE score** (S_{rmse})
    - **Phase shift** and **seasonal cycle score** (S_{phase})
    - **Interannual coefficient of variation** and **IAV score** (S_{iav})
    - **Spatial distribution score** (S_{dist})
    - **Overall score** (S_{overall})

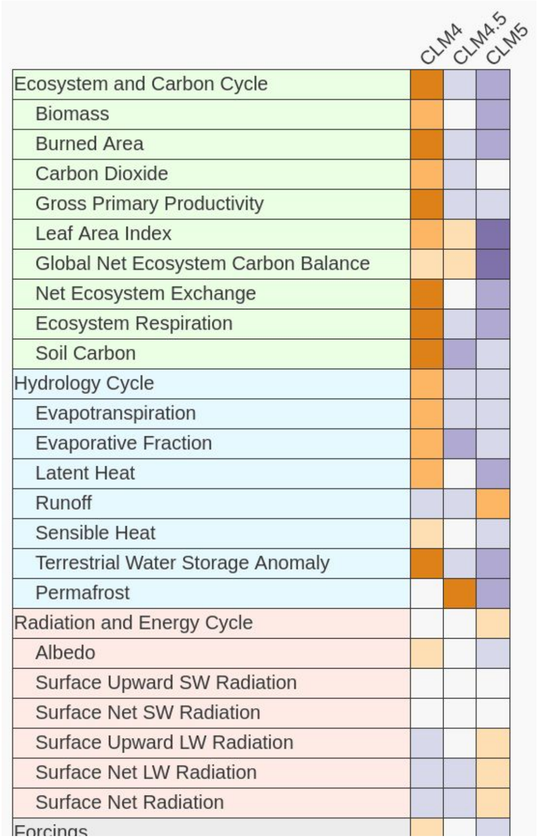
$$S_{\text{overall}} = \frac{S_{\text{bias}} + 2S_{\text{rmse}} + S_{\text{phase}} + S_{\text{iav}} + S_{\text{dist}}}{1+2+1+1+1}$$

  - **Graphical diagnostics**
    - Spatial contour maps
    - Time series line plots
    - Spatial Taylor diagrams (Taylor, 2001)
- Similar **tables** and **graphical diagnostics** for functional relationships

ILAMB Current Variables

- **Biogeochemistry:** Biomass (Contiguous US, Pan Tropical Forest), Burned area (GFED3), CO_2 (NOAA GMD, Mauna Loa), Gross primary production (Fluxnet, GBAF), Leaf area index (AVHRR, MODIS), Global net ecosystem carbon balance (GCP, Khatiwala/Hoffman), Net ecosystem exchange (Fluxnet, GBAF), Ecosystem Respiration (Fluxnet, GBAF), Soil C (HWSD, NCSCDv22, Koven)
- **Hydrology:** Evapotranspiration (GLEAM, MODIS), Evaporative fraction (GBAF), Latent heat (Fluxnet, GBAF, DOLCE), Runoff (Dai, LORA), Sensible heat (Fluxnet, GBAF), Terrestrial water storage anomaly (GRACE), Permafrost (NSIDC)
- **Energy:** Albedo (CERES, GEWEX.SRB), Surface upward and net SW/LW radiation (CERES, GEWEX.SRB, WRMC.BSRN), Surface net radiation (CERES, Fluxnet, GEWEX.SRB, WRMC.BSRN)
- **Forcing:** Surface air temperature (CRU, Fluxnet), Diurnal max/min/range temperature (CRU), Precipitation (CMAP, Fluxnet, GPCC, GPCP2), Surface relative humidity (ERA), Surface down SW/LW radiation (CERES, Fluxnet, GEWEX.SRB, WRMC.BSRN)

ILAMB Assessing Multiple Generations of CLM

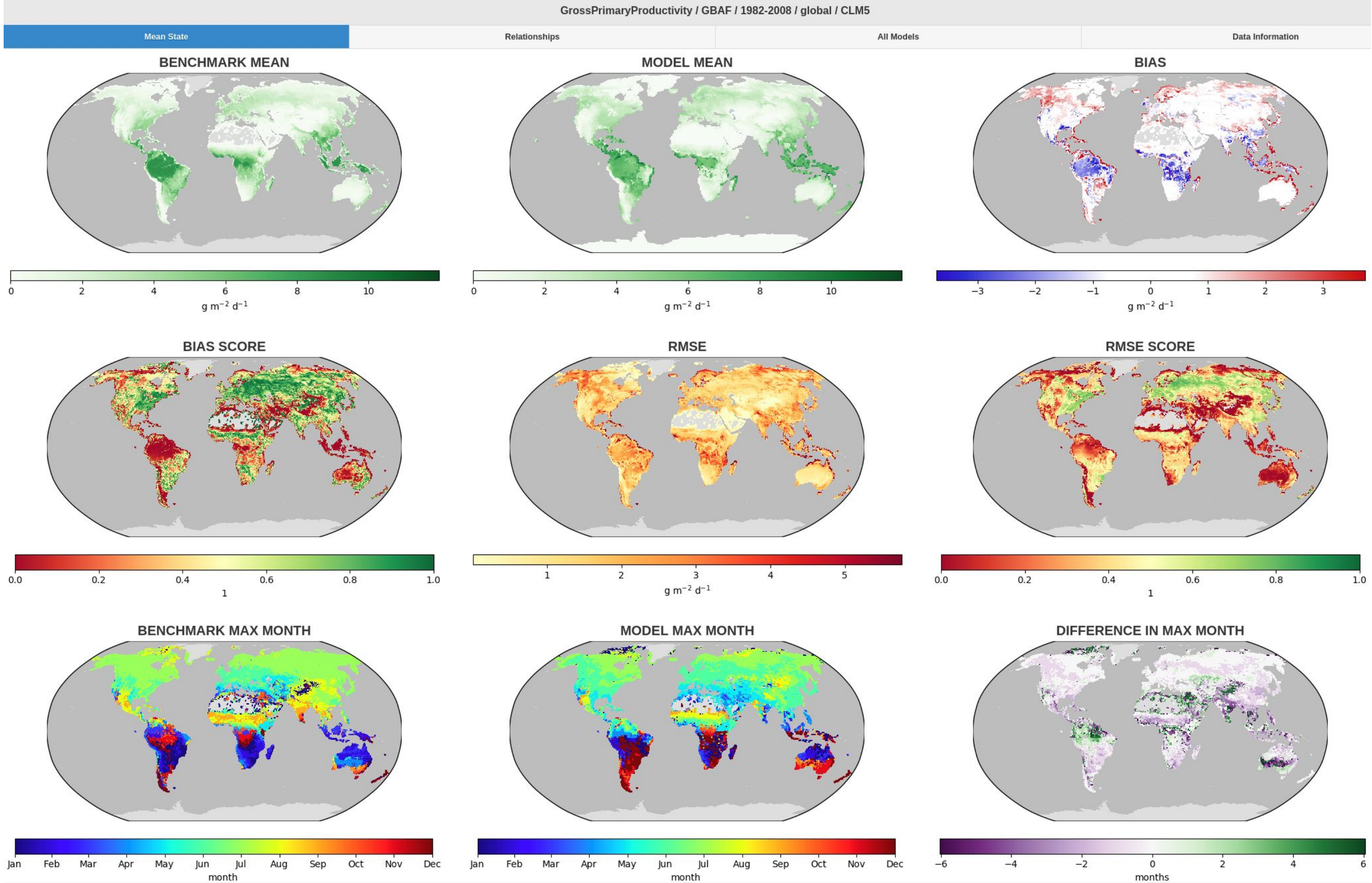


- Improvements in mechanistic treatment of hydrology, ecology, and land use with much more complexity in Community Land Model version 5 (CLM5)
- Simulations improved even with enhanced complexity
- Observational datasets not always self-consistent
- Forcing uncertainty confounds assessment of model development

http://webext.cgd.ucar.edu/I20TR/_build_set1F/

(Lawrence et al., 2019)

ILAMB Graphical Diagnostics



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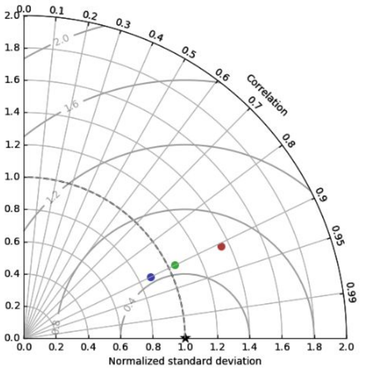
ILAMB Graphical Diagnostics

RUBISCO

SPATIAL TAYLOR DIAGRAM



MODEL COLORS

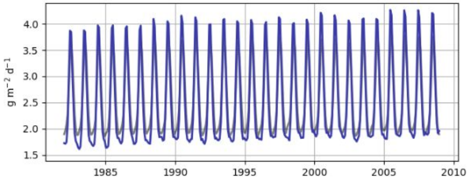
- Benchmark
- CLM4
- CLM4.5
- CLM5

Spatially integrated regional mean

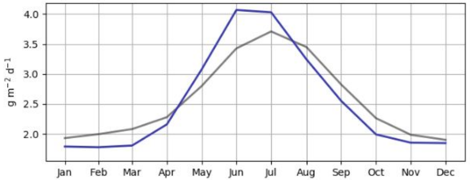
MODEL COLORS

- Benchmark
- CLM4
- CLM4.5
- CLM5

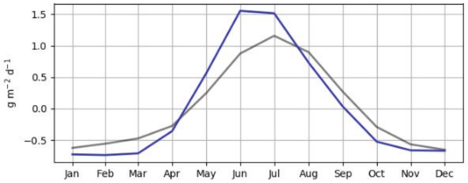
REGIONAL MEAN



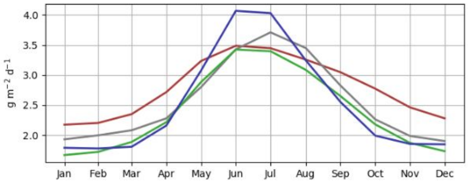
ANNUAL CYCLE



MONTHLY ANOMALY



ANNUAL CYCLE

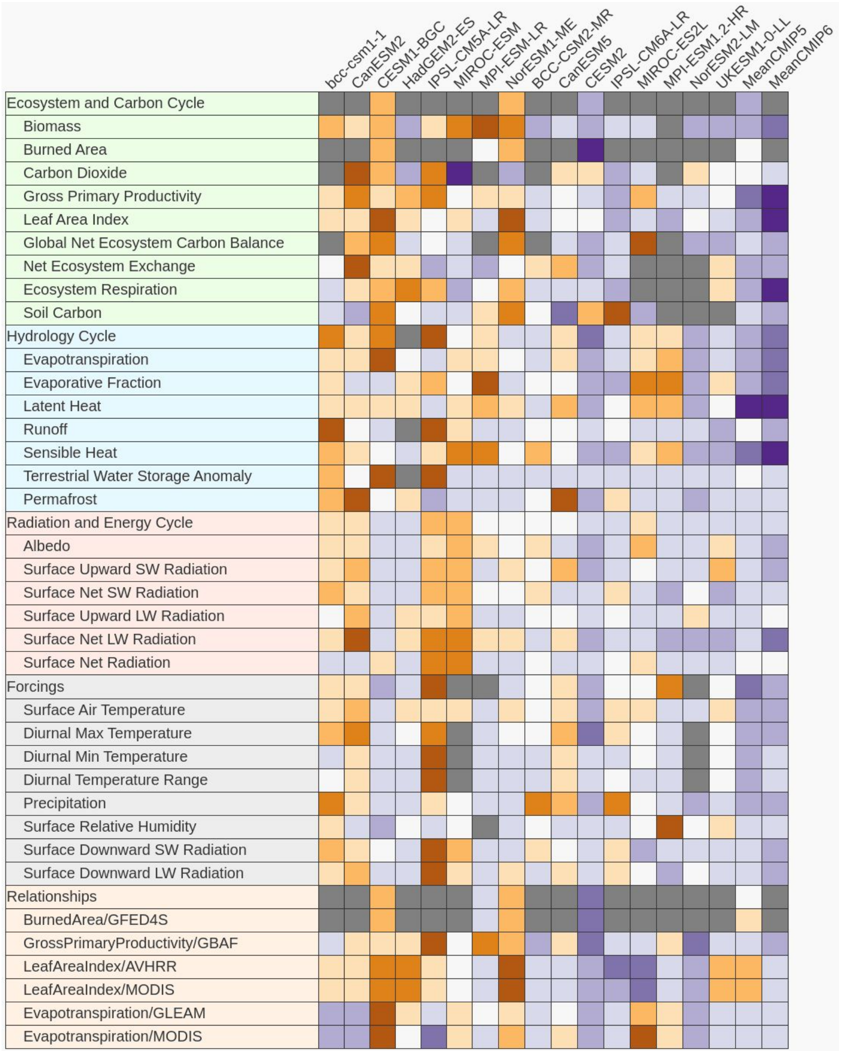


BERKELEY LAB · NCAR NATIONAL CENTER FOR ATMOSPHERIC RESEARCH · OAK RIDGE National Laboratory · Sandia National Laboratories · THE UNIVERSITY OF CALIFORNIA IRVINE · MICHIGAN

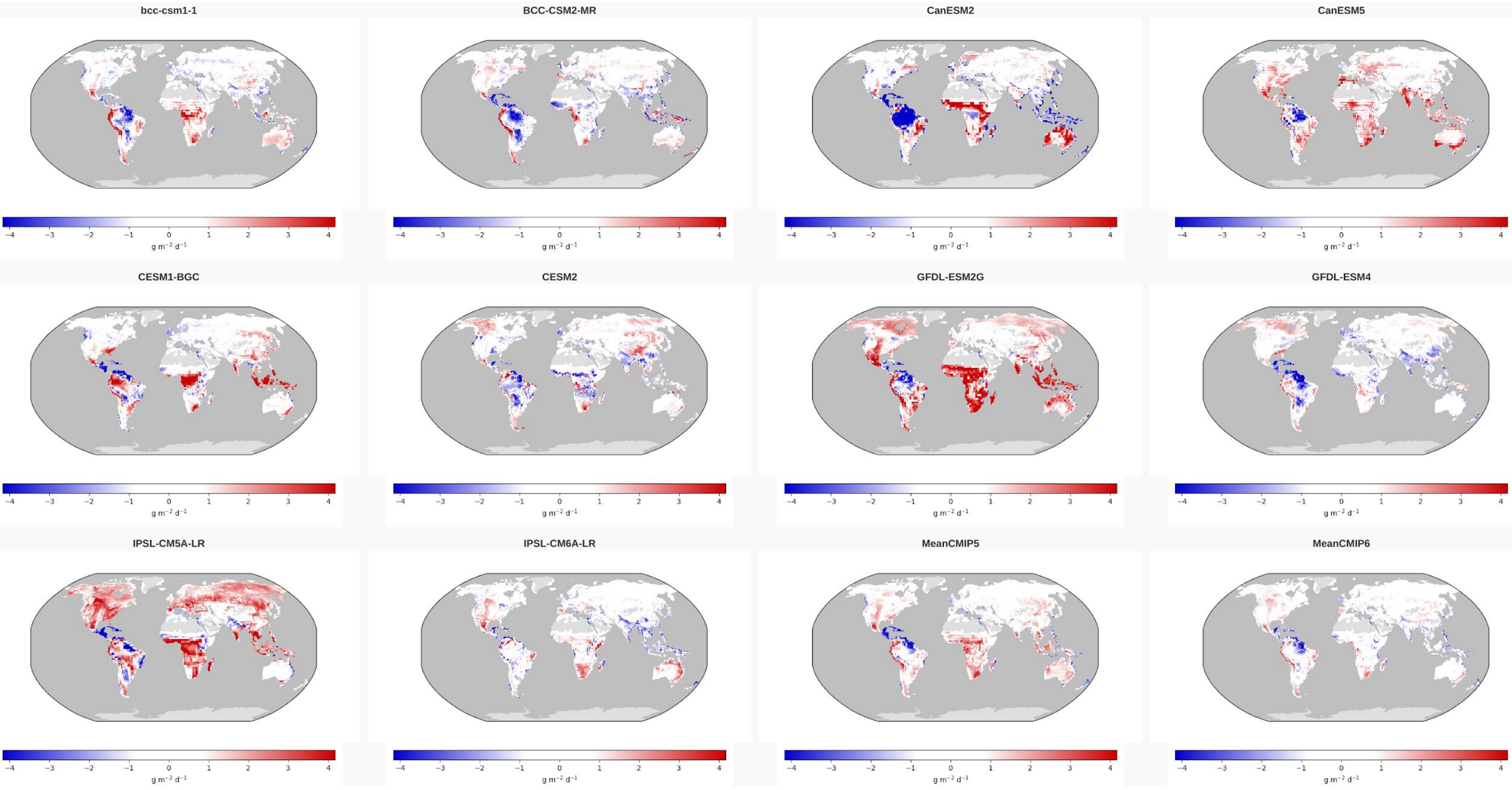
RUBISCO

CMIP5 vs. CMIP6 Models

- The CMIP6 suite of land models (right) has improved over the CMIP5 suite of land models (left)
- The multi-model mean outperforms any single model for each suite of models
- The multi-model mean CMIP6 land model is the “best model” overall
- Why did CMIP6 land models improve?



(Hoffman et al., in prep)

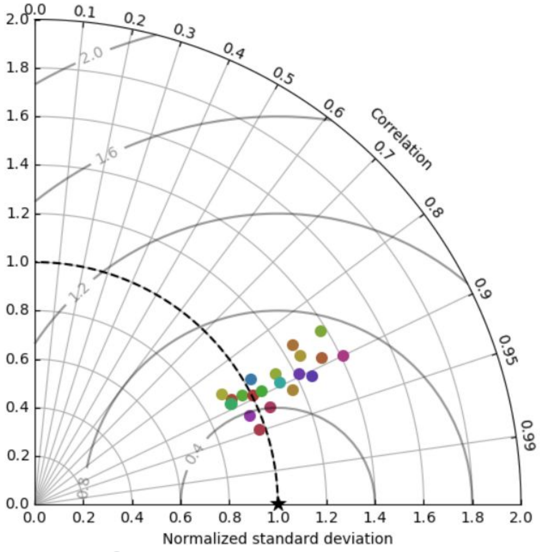

bcc-csm1-1
BCC-CSM2-MR
CanESM2
CanESM5
CESM1-BGC
CESM2
GFDL-ESM2G
GFDL-ESM4
IPSL-CM5A-LR
IPSL-CM6A-LR
MeanCMIP5
MeanCMIP6
−4 −3 −2 −1 0 1 2 3 4
g m−2 d−1

Gross Primary Productivity

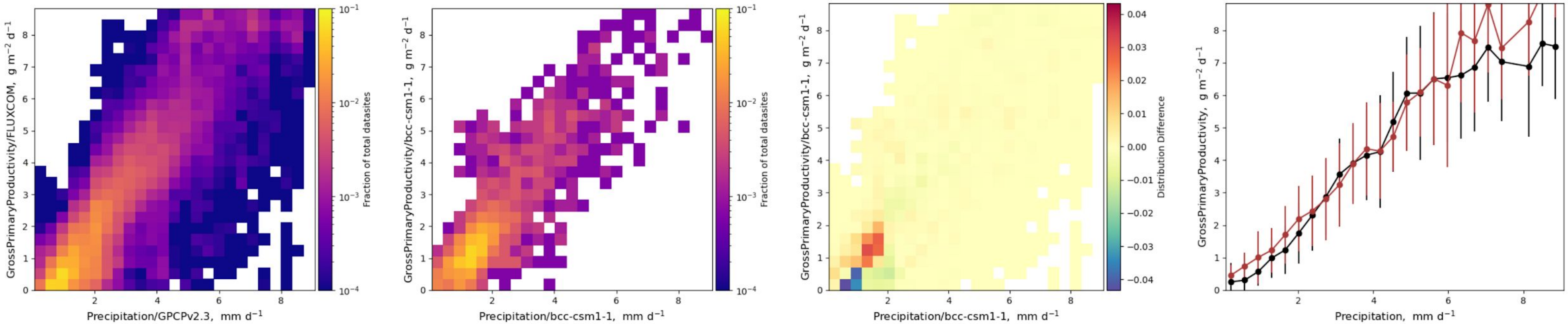
	Download Data	Period Mean (original grids) [Pg yr-1]	Model Period Mean (intersection) [Pg yr-1]	Benchmark Period Mean (intersection) [Pg yr-1]	Model Period Mean (complement) [Pg yr-1]	Benchmark Period Mean (complement) [Pg yr-1]	Bias [g m-2 d-1]	RMSE [g m-2 d-1]	Phase Shift [months]	Bias Score [1]	RMSE Score [1]	Seasonal Cycle Score [1]	Spatial Distribution Score [1]	Overall Score [1]
Benchmark	[-]	114.												
bcc-csm1-1	[-]	123.	112.	114.	8.79	0.0945	0.238	1.51	1.01	0.484	0.435	0.830	0.955	0.628
BCC-CSM2-MR	[-]	114.	107.	113.	5.88	0.671	-0.0233	1.52	1.11	0.479	0.447	0.817	0.941	0.626
CanESM2	[-]	129.	117.	114.	9.54		0.0601	2.31	2.00	0.388	0.437	0.650	0.836	0.549
CanESM5	[-]	141.	128.	114.	10.1		0.730	1.87	1.60	0.449	0.418	0.710	0.948	0.589
CESM1-BGC	[-]	129.	123.	113.	5.55	0.660	0.379	1.66	1.20	0.426	0.468	0.765	0.889	0.603
CESM2	[-]	110.	104.	113.	5.57	0.642	-0.0542	1.62	1.32	0.458	0.466	0.774	0.933	0.619
GFDL-ESM2G	[-]	167.	152.	114.	12.4		1.26	2.78	1.38	0.377	0.288	0.735	0.897	0.517
GFDL-ESM4	[-]	105.	99.0	114.	6.18		-0.177	1.59	1.49	0.495	0.403	0.702	0.939	0.588
IPSL-CM5A-LR	[-]	165.	150.	113.	11.7	0.515	1.18	2.68	1.20	0.327	0.352	0.781	0.896	0.542
IPSL-CM6A-LR	[-]	115.	109.	113.	5.27	0.708	0.111	1.39	1.14	0.547	0.477	0.790	0.961	0.650
MeanCMIP5	[-]	121.	115.	114.	6.65		0.574	1.41	0.981	0.494	0.502	0.799	0.965	0.652
MeanCMIP6	[-]	116.	110.	114.	6.26		0.129	1.17	0.931	0.572	0.522	0.826	0.956	0.679
MIROC-ESM	[-]	129.	118.	102.	9.04	11.4	0.396	1.90	1.27	0.463	0.435	0.767	0.920	0.604
MIROC-ESM2L	[-]	116.	104.	113.	9.90	0.119	-0.0111	1.95	1.99	0.409	0.379	0.628	0.920	0.543
MPI-ESM-LR	[-]	169.	159.	104.	8.91	9.81	1.36	2.36	1.29	0.402	0.371	0.715	0.930	0.558
MPI-ESM1.2-LR	[-]	141.	133.	104.	6.89	9.81	0.725	2.06	1.13	0.409	0.393	0.769	0.925	0.578
NorESM1-ME	[-]	129.	120.	114.	7.82		0.386	1.86	1.25	0.387	0.456	0.761	0.856	0.583
NorESM2-LM	[-]	107.	97.5	114.	7.59		-0.0828	1.63	1.31	0.443	0.472	0.791	0.938	0.623
UK-HadGEM2-ES	[-]	137.	130.	113.	6.93	0.848	0.602	2.01	1.10	0.389	0.388	0.820	0.855	0.568
UKESM1-0-LL	[-]	126.	119.	113.	7.06	0.825	0.387	1.77	1.16	0.436	0.419	0.791	0.924	0.598

- Multimodel GPP is compared with global seasonal GBAF estimates
- We can see Improvements across generations of models (e.g., CESM1 vs. CESM2, IPSL-CM5A vs. 6A)
- The mean CMIP6 and CMIP5 models perform best

Spatial Taylor Diagram



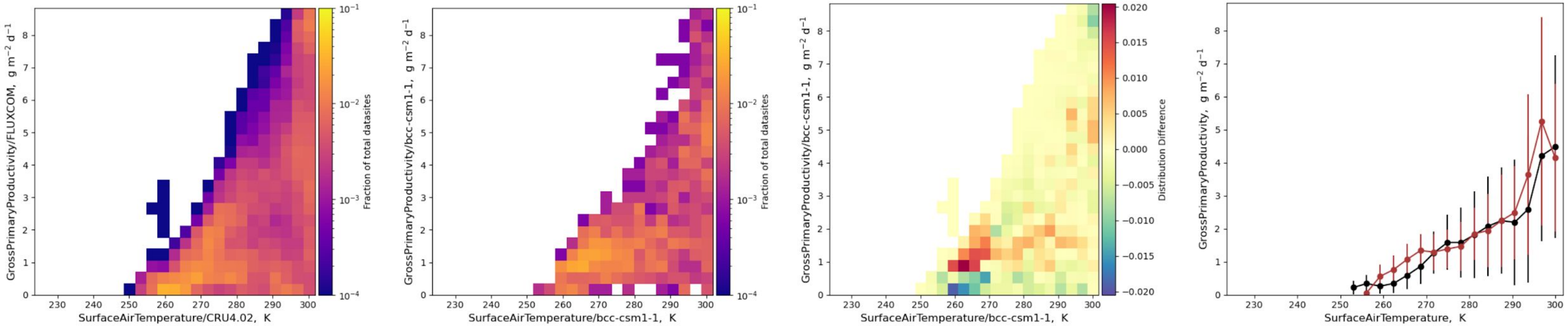
Precipitation/GPCPv2.3



SurfaceDownwardSWRadiation/CERESed4.1

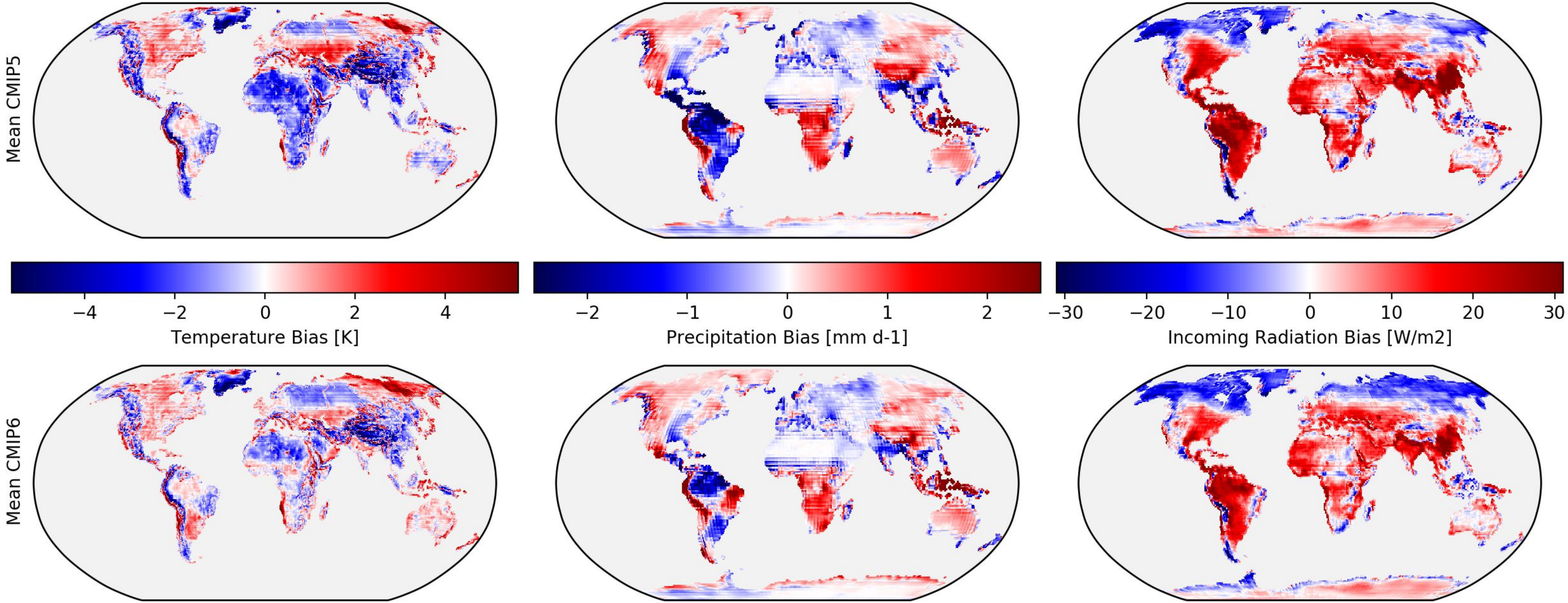
SurfaceNetSWRadiation/CERESed4.1

SurfaceAirTemperature/CRU4.02



Reasons for Land Model Improvements

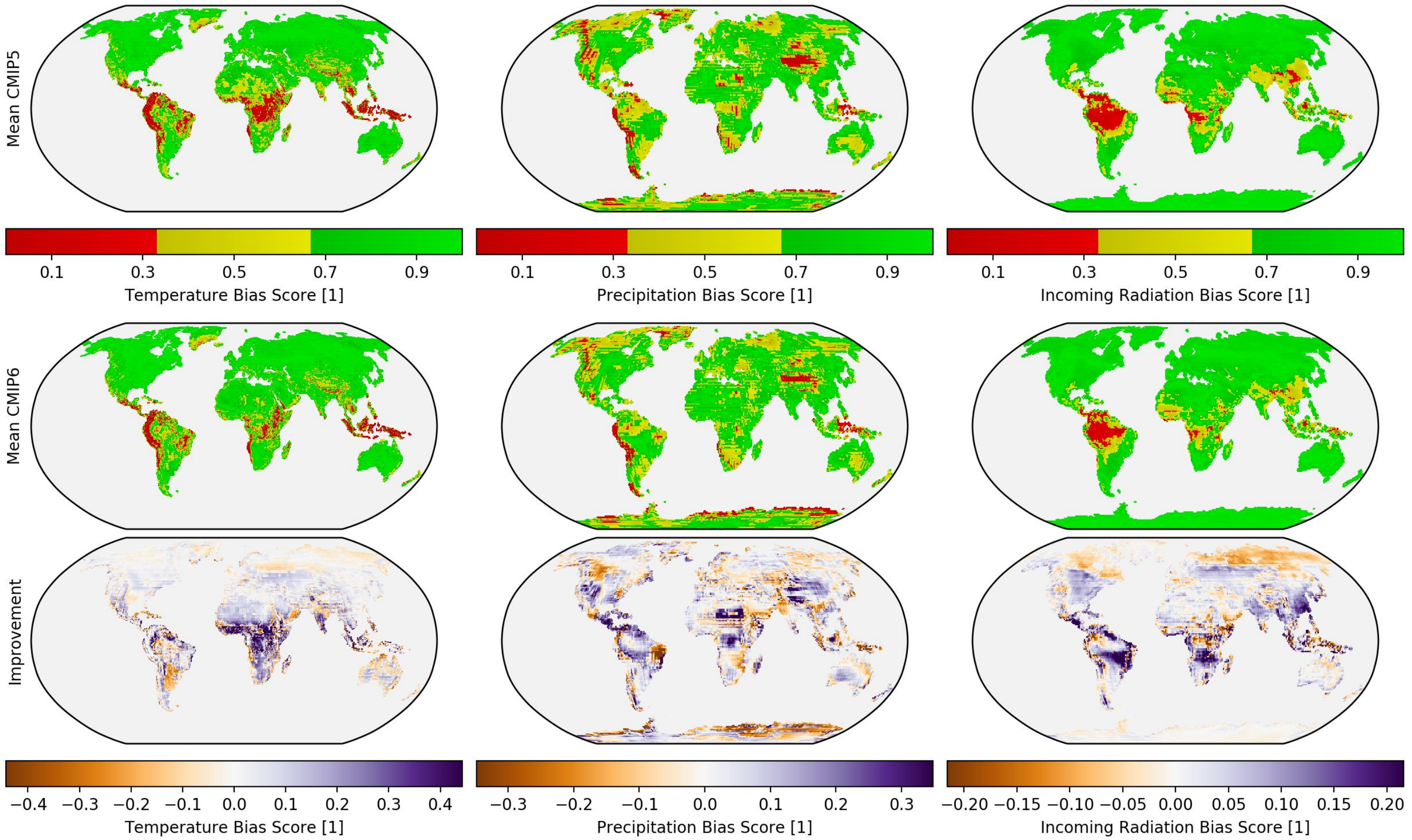
ESM improvements in climate forcings (temperature, precipitation, radiation) likely partially drove improvements exhibited by land carbon cycle models



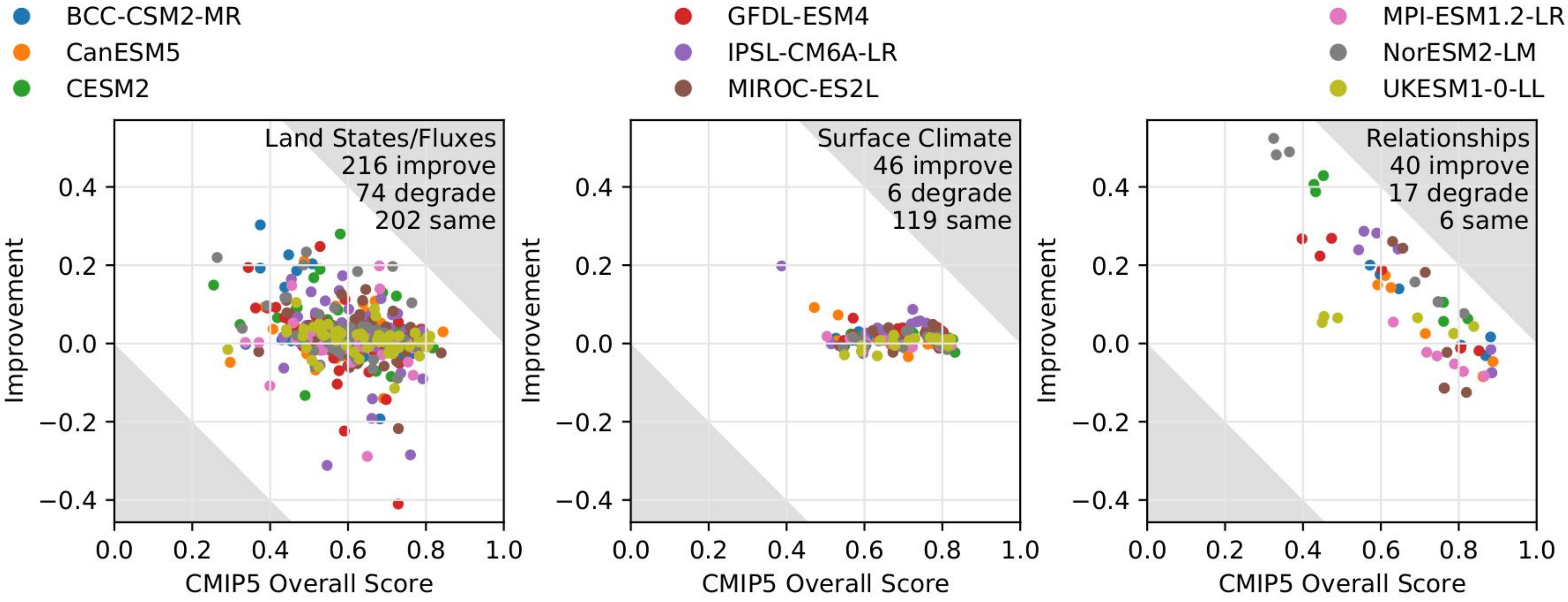
(Hoffman et al., in prep)

Reasons for Land Model Improvements

Differences in bias scores for temperature, precipitation, and incoming radiation were primarily positive, further indicating more realistic climate representation



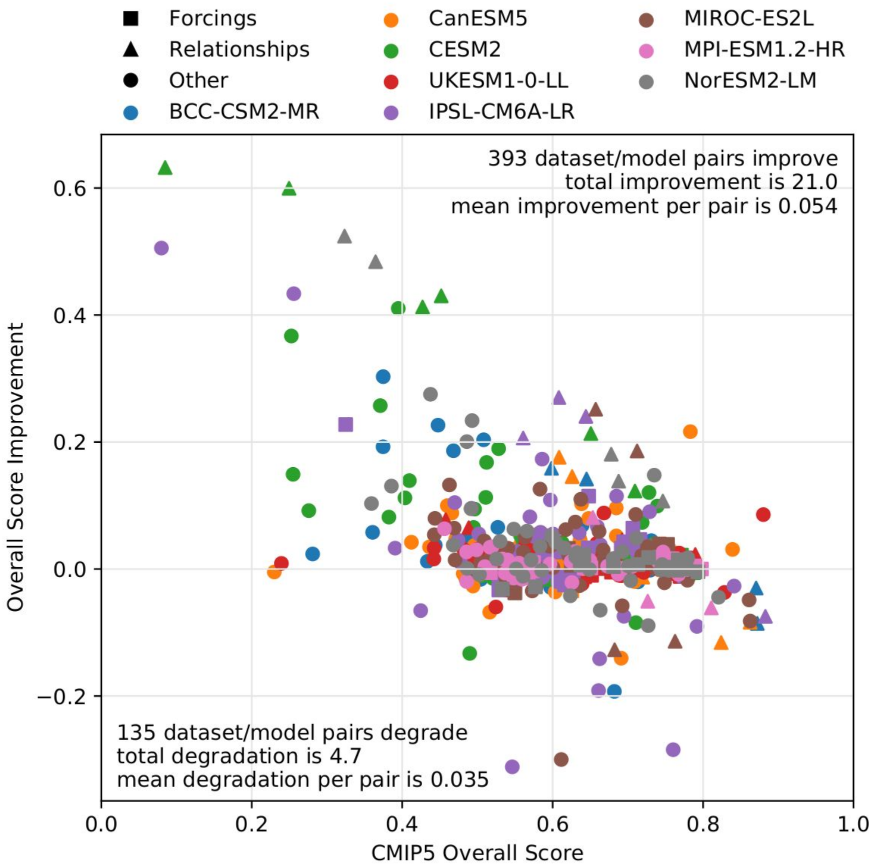
(Hoffman et al., in prep)



Across all land models, scores for most state and flux variables improved (216) or remained nearly the same (202), although some were degraded (74). While atmospheric forcings from CMIP6 ESMs were improved over those from CMIP5 ESMs, the largest improvements were in land model **variable-to-variable relationships**, suggesting that increased land model development was also partially responsible for higher CMIP6 land model scores.

Reasons for Land Model Improvements

While forcings got better, the largest improvements were in **variable-to-variable relationships**, suggesting that increased land model complexity was also partially responsible for higher CMIP6 model scores



ILAMB & IOMB CMIP5 vs 6 Evaluation

RUBISCO

- (a) ILAMB and (b) IOMB have been used to evaluate how land and ocean model performance have changed from CMIP5 to CMIP6
- Model fidelity is assessed through comparison of historical simulations with a wide variety of contemporary observational datasets
- The UN's Intergovernmental Panel on Climate Change (IPCC) Sixth Assessment Report (AR6) from Working Group 1 (WG1) Chapter 5 contains the full ILAMB/IOMB evaluation as Figure 5.22

	CMIP5 ESMs									CMIP6 ESMs										
	bcc-csm1-1	CanESM2	CESM1-BGC	GFDL-ESM2G	IPSL-CM5A-LR	MIROC-ESM	MPI-ESM-LR	NorESM1-ME	HadGEM2-ES	BCC-CSM2-MR	CanESM5	CESM2	GFDL-ESM4	IPSL-CM6A-LR	MIROC-ES2L	MPI-ESM1.2-LR	NorESM2-LM	UKESM1-0-LL	Mean CMIP5	Mean CMIP6
(a) Land Benchmarking Results																				
Land Ecosystem & Carbon Cycle	-0.72	-0.93	-1.55	-1.51	-0.13	0.60	-0.43	-1.31	0.19	-0.43	0.66	0.48	-1.09	0.22	0.60	-0.07	1.00	0.49	1.63	2.30
Biomass	0.20	-0.45	-1.52	-0.40	-1.26	-0.26	-1.07	-1.77	0.92	1.39	0.74	-0.20	-0.54	0.16	0.93	-0.96	-0.01	1.04	1.23	1.82
Burned Area			-0.87				0.10	-0.83				1.60								
Leaf Area Index	-0.20	-0.64	-1.30	-2.53	-0.01	0.30	0.01	-1.85	-0.16	0.27	0.08	0.34	-0.70	1.19	0.82	0.46	0.37	0.69	1.04	1.81
Soil Carbon	0.27	1.26	-1.46	0.07	0.75	0.47	-0.03	-1.14	0.07	0.23	1.35	-0.99	-2.04	-1.55	0.90	-0.75	-0.17	0.24	1.01	1.48
Gross Primary Productivity	0.59	-1.23	0.01	-1.81	-1.40	0.29	-0.53	-0.24	-1.04	0.77	0.04	0.59	-0.38	1.17	-1.02	-0.37	0.73	0.09	1.51	2.22
Net Ecosystem Exchange	-0.42	-1.81	-0.21	-0.65	1.10	-0.24	0.80	0.02	-1.03	-1.02	-1.19	0.59	1.69	-0.42	0.63	-0.21	1.08	-1.43	1.28	1.43
Ecosystem Respiration	0.90	-0.56	-0.86	-0.24	-1.35	0.99	-0.01	-0.94	-1.54	0.81	0.59	0.51	-0.79	0.90	-0.21	-1.24	0.43	-0.94	1.34	2.21
Carbon Dioxide		-1.54	-0.36	-2.92	-0.74	1.53	-0.00	0.37	0.85		0.42	0.26	0.39	0.59	1.10	-0.87	0.21	0.69	0.09	-0.07
Global Net Carbon Balance		-1.64	-0.88	-1.13	0.17	-0.31	-0.38	-0.50	0.24		-0.23	1.34	-1.70	0.17	-0.74	1.45	1.56	0.26	0.92	1.40
Land Hydrology Cycle	-2.65	-0.42	0.44	-0.18	-0.49	-0.52	-0.57	0.17	0.70	0.15	-0.47	1.51	-1.24	0.58	-0.72	-0.83	0.97	0.87	1.00	1.70
Evapotranspiration	-0.82	-0.99	-0.27	-1.02	0.64	-1.14	-0.62	-0.60	0.28	0.39	-1.08	1.09	0.65	0.43	-1.40	-1.01	0.82	1.05	1.41	2.20
Evaporative Fraction	-0.34	0.74	0.74	-0.14	-0.85	0.21	-1.98	0.22	-0.34	0.10	0.11	1.25	-0.88	1.29	-1.65	-1.81	1.11	-0.06	0.98	1.29
...																				
Terrestrial Water Storage Anomaly	-2.79	-0.45	0.47	0.50	-0.38	0.34	0.35	0.43	0.58	0.15	-0.08	0.95	-2.91	0.43	0.37	0.15	0.39	0.51	0.49	0.50
Permafrost	-0.88	-2.26	0.01	0.13	0.83	0.69	0.56	0.69	-0.56	-0.11	-3.02	0.83	0.74	-0.18	0.49	0.42	0.89	0.43	0.06	0.23
(b) Ocean Benchmarking Results																				
Ocean Ecosystems			2.18	0.20	-0.20		0.04		0.22		-0.37	0.83	-0.37	-0.26	-0.91	-0.67	-1.93	0.27	0.30	0.67
Chlorophyll		-1.50	2.15	0.44	1.02		0.49		0.56		-0.67	0.88	-0.21	0.10	-1.02	-0.41	-2.19	0.18	0.13	0.04
Oxygen, surface			0.73	-0.13	-1.98		-0.53	-1.53	-0.29		0.73	0.34	-0.09	-0.41	0.35	-0.30	0.40	0.49	0.64	1.57
Ocean Nutrients			-0.84	-0.10	0.91		-0.80	-1.25				-0.02	1.00	1.88		-0.90	-1.14	-0.17	-0.16	1.60
Nitrate, surface		0.21	-1.63	0.67	1.22		-0.18	-1.70	0.82		1.21	-0.90	0.29	1.21	1.02	0.39	-1.78	-0.56	-0.47	0.18
Phosphate, surface			-0.69	-0.04	0.04		-0.45	-0.43				0.39	-0.14	0.17	-0.41	-0.98	0.00	0.02	0.88	1.63
Silicate, surface			0.44	-0.71	0.24		-0.81	-0.20	-2.16			0.50	1.24	1.60		-1.21	-0.19	0.18	-0.29	1.37
Ocean Carbon											1.24	-0.23	-0.62	-0.69	-1.08	-1.12	1.31			1.19
TAlk, surface		-0.27	1.01	0.12	0.19		0.32	-2.31	-0.22		0.06	-0.36	0.85	-0.42	0.29	-2.40	1.27	0.06	1.27	0.54
...																				
Salinity, 700m	0.44	-0.35	-1.06	-0.54	0.70	0.46	-0.46	-0.80	0.32	0.36	0.25	-1.16	-0.47	0.54	0.33	-0.39	-0.87	-0.54	1.58	1.64
Ocean Relationships			-1.86	-0.36	-0.29		1.50	-0.43	0.68		-0.02	0.72	1.20	0.17	-1.86	0.02		-1.12	0.39	1.25
Oxygen, surface/WOA2018			0.27	0.23	-0.63		-0.26	-0.12	-0.38		0.29	-0.21	0.19	0.18	0.14	-0.07		0.03	-0.23	0.53
Nitrate, surface/WOA2018		-2.41	-1.38	-0.18	0.06		1.41	-0.16	0.78		0.09	0.79	1.07	0.26	-1.35	0.20		-0.74	0.52	1.04

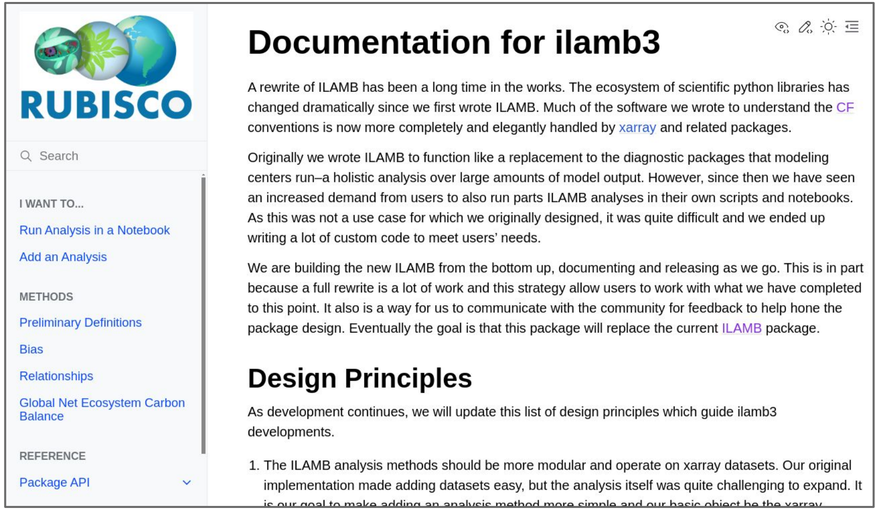
Relative Scale

Worse Value **Better Value**

Missing Data or Error

ILAMBv3: Ongoing Development

- Continuously updated documentation as new modules are being developed: https://ilamb3.readthedocs.io/



Documentation for ilamb3

A rewrite of ILAMB has been a long time in the works. The ecosystem of scientific python libraries has changed dramatically since we first wrote ILAMB. Much of the software we wrote to understand the CF conventions is now more completely and elegantly handled by xarray and related packages.

Originally we wrote ILAMB to function like a replacement to the diagnostic packages that modeling centers run–a holistic analysis over large amounts of model output. However, since then we have seen an increased demand from users to also run parts ILAMB analyses in their own scripts and notebooks. As this was not a use case for which we originally designed, it was quite difficult and we ended up writing a lot of custom code to meet users' needs.

We are building the new ILAMB from the bottom up, documenting and releasing as we go. This is in part because a full rewrite is a lot of work and this strategy allow users to work with what we have completed to this point. It also is a way for us to communicate with the community for feedback to help hone the package design. Eventually the goal is that this package will replace the current ILAMB package.

Design Principles

As development continues, we will update this list of design principles which guide ilamb3 developments.

1. The ILAMB analysis methods should be more modular and operate on xarray datasets. Our original implementation made adding datasets easy, but the analysis itself was quite challenging to expand. It


```
In [2]: import matplotlib.pyplot as plt
        import ilamb3
        from ilamb3.analysis import bias_analysis
```

Initialize an analysis, specifying the variable name to be compared.

```
In [3]: analysis = bias_analysis("biomass")
```

Load two ILAMB data products using a built-in catalog

```
In [4]: cat = ilamb3.ilamb_catalog()
        ds_esacci = cat["biomass | ESACCI"].read()
        ds_xu = cat["biomass | XuSaatchi2021"].read()
```

Apply the analysis using the ESACCI product as a reference.

```
In [5]: df,ds_esacci,ds_xu = analysis(ds_esacci,ds_xu)
```

```
In [6]: df
```

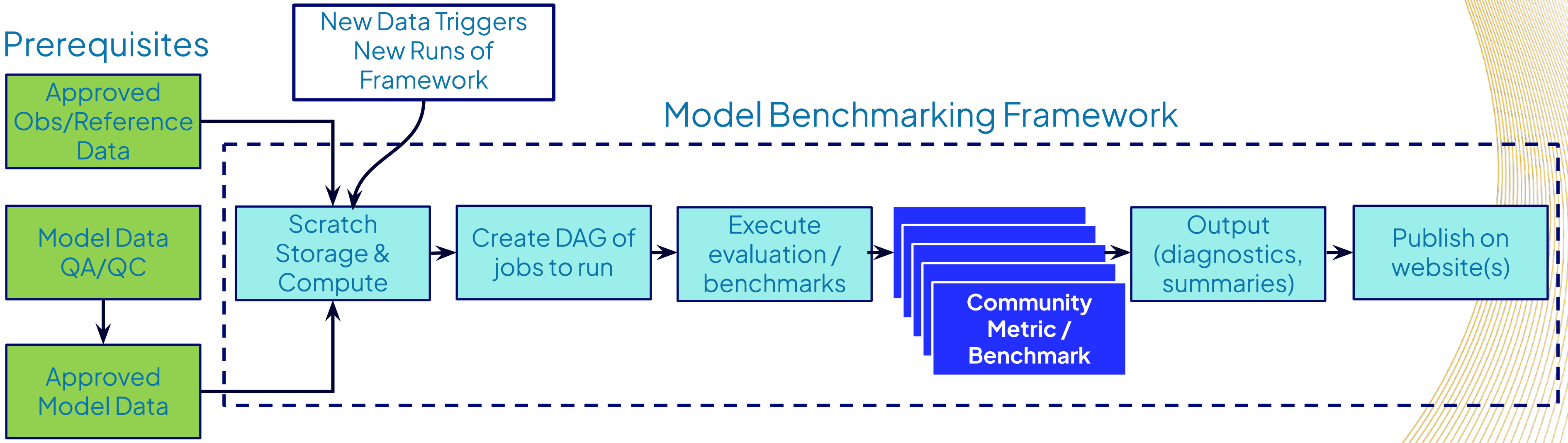
Out[6]:

	source	region	analysis	name	type	units	value
0	Reference	None	Bias	Period Mean	scalar	Mg ha-1	24.019928
1	Comparison	None	Bias	Period Mean	scalar	Mg ha-1	25.676543
2	Comparison	None	Bias	Bias	scalar	Mg ha-1	-16.670597
3	Comparison	None	Bias	Bias Score	score	1	0.398491

- ILAMBv3 allows for analysis methods to be imported into Python scripts and Jupyter notebooks and used to produce the scalars and plots synthesized in the full analysis
- At left, the ILAMB bias analysis is applied to two reference data products and show a table of scalar values

CMIP Rapid Evaluation Framework Overview

The Coupled Model Intercomparison Project (CMIP) Model Benchmarking Task Team developed a system specification for a Rapid Evaluation Framework (REF) that would leverage community benchmarking metrics to evaluate CMIP model output as they are submitted to the Earth System Grid Federation (ESGF)



CMIP Benchmarking Task Team – Birgit Hassler, Forrest Hoffman, & Ranjini Swaminathan, Co-leads

Find out more about the CMIP Rapid Evaluation Framework (REF)

The CMIP AR7 Fast Track Rapid Evaluation Framework (AR7 FT REF) will be a complete end to end system providing a systematic and rapid performance assessment of the expected models participating in the CMIP AR7 Fast Track, supporting the next IPCC Assessment Report 7 (AR7) cycle.

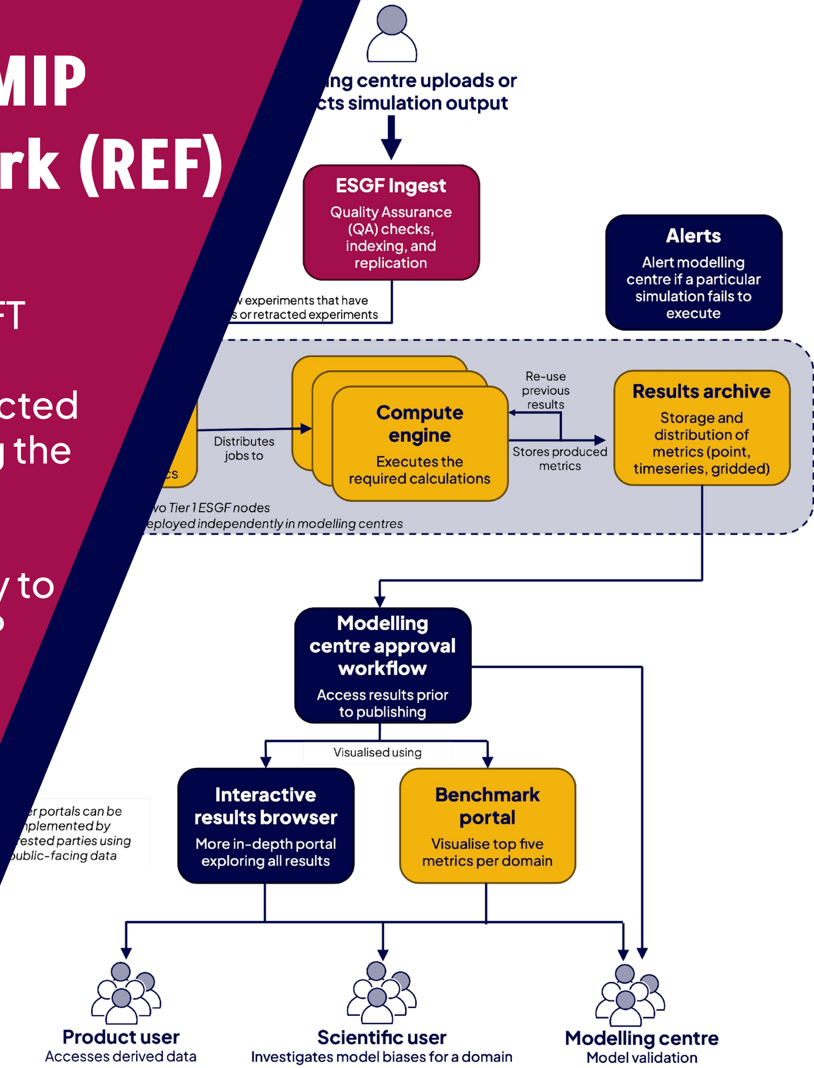
The REF is designed to be a starting point for the community to develop and build upon, with applications across the WCRP and beyond.

Find out more at
wcrp-cmip.org/cmip7/rapid-evaluation-framework/

This project has been made possible by funding from:

U.S. DEPARTMENT of ENERGY

esa



Key Links

- Repository: https://github.com/rubisco-sfa/ilamb3
- Documentation [outdated]: https://ilamb3.readthedocs.io/en/latest/
- Sample output:
  - Land: https://www.ilamb.org/dev/Land/index.html
  - Ocean: https://www.ilamb.org/dev/Ocean/index.html
- Data preparation: https://github.com/rubisco-sfa/ilamb3-data
- Climate-REF: https://github.com/Climate-REF/climate-ref

Summary

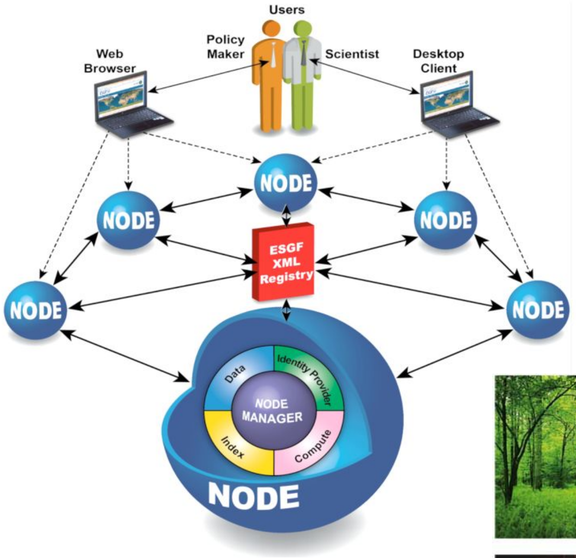
- **Model benchmarking** is increasingly important as model complexity increases
- Systematic model benchmarking is useful for
    - **Verification** – during model development to confirm that new model code improves performance in a targeted area without degrading performance in another area
    - **Validation** – when comparing performance of one model or model version to observations and to other models or other model versions
- The **ILAMB package** employs a suite of in situ, remote sensing, and reanalysis datasets to comprehensively evaluate and score land model performance, *irrespective of any model structure or set of process representations*
- ILAMB is **Open Source**, is written in **Python**, **runs in parallel** on laptops to supercomputers, and has been **adopted in many modeling centers and MIPs**
- The *usefulness* of ILAMB depends on the quality of incorporated observational data, characterization of uncertainty, and selection of relevant metrics

Earth System Grid Federation (ESGF)

What is the Earth System Grid Federation?

- **Earth System Grid Federation (ESGF)** is an *international consortium* and a *globally distributed network of data servers* using a common set of protocols & interfaces to archive and distribute Earth system model output and related input, observational, and reanalysis data
- These **Open Science data** are used by scientists all over the world to investigate Earth system variability and feedbacks and to inform research and assessments

ESGF Conceptual Diagram



ESGF
Earth System Grid Federation

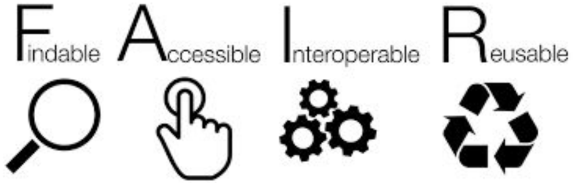
Data are now being used to ***train Artificial Intelligence (AI) models*** *to predict Earth system processes*

ESGF data offer insights into key Earth system interactions among the land, ocean, and atmosphere

Logos represent primary international contributors: US Department of Energy, NASA, NOAA, NSF, European IS-ENES Project, and Australian NCI

ESGF Holdings are Large and Open

- CMIP5 totals >1.5 PB (>5 PB including replicas)
- CMIP6 totals >16.1 PB (>27 PB including replicas)
- CMIP7 is expected to have more experiments, high resolution output, and ensembles, totaling 80–100 PB



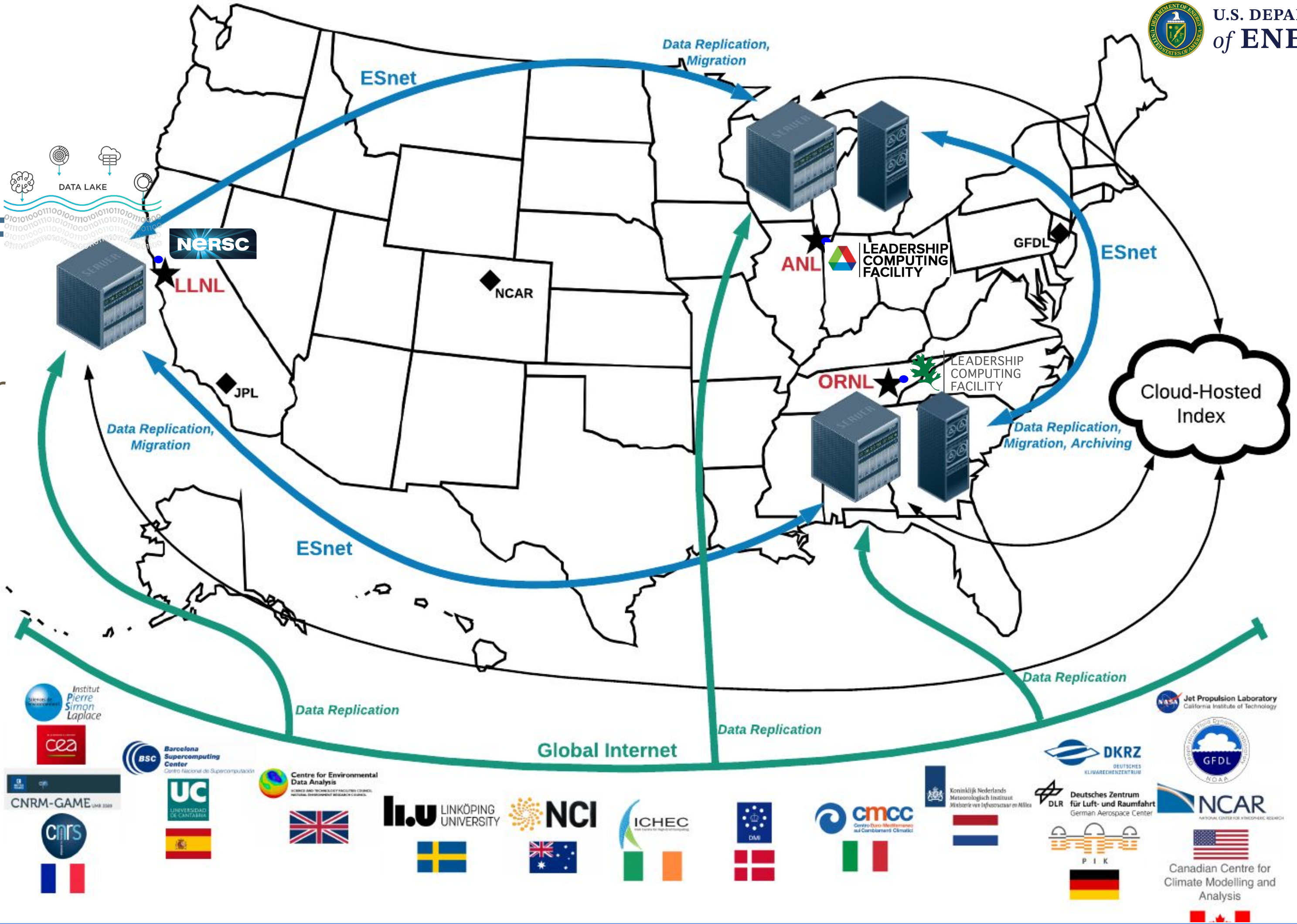
- ESGF is concerned with the *full stack security* and the *integrity of data*, but we are **not** concerned about limiting *access to data*
- ESGF is a **DOE ASCR Integrated Research Infrastructure (IRI)** Pathfinder project

Project	Total	Distinct	Replica
CMIP6	14,893,892 total datasets 27,983.73 TB	7,670,309 distinct datasets 16,120.41 TB	7,223,583 replica datasets 11,863.32 TB
CORDEX	187,785 total datasets 1,473.33 TB	187,513 distinct datasets 1,472.77 TB	272 replica datasets 0.56 TB
CMIP5	201,130 total datasets 5,293.61 TB	52,163 distinct datasets 1,525.07 TB	148,967 replica datasets 3,768.55 TB
INPUT4MIPS	5,871 total datasets 10.84 TB	21 distinct datasets 0.9 TB	5,850 replica datasets 9.95 TB
OBS4MIPS	126 total datasets 0.2 TB	108 distinct datasets 0.2 TB	18 replica datasets 0.01 TB

As of April 7, 2025

DOE's Next Generation ESGF

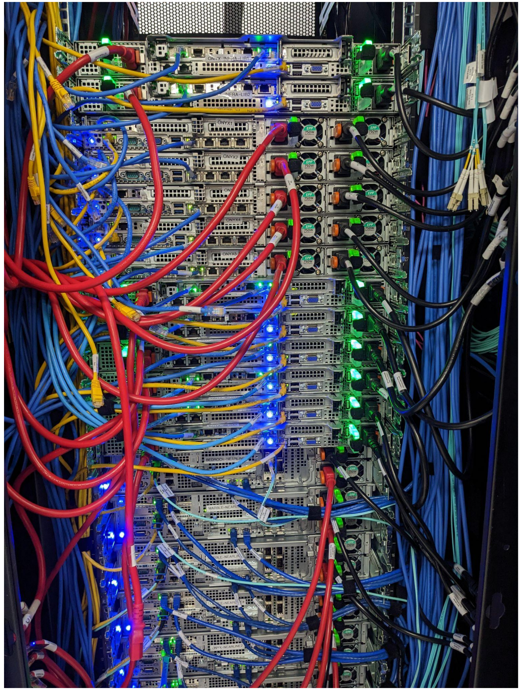
- As many as 3 nodes located at DOE's major computing facilities
- Replicating data from the worldwide Federation
- Providing scalable cloud indexing and tape archiving



ESGF2 US Data and Index Nodes Deployed at ORNL

- Containerized server software deployed on the shared Onyx cluster is serving 8 PB of Coupled Model Intercomparison Project (CMIP5 and CMIP6) data at ORNL
- Data are stored on the new Themis hierarchical storage platform, providing on-disk copy for fast access to frequently used data and backup copies on two tapes for all data
- Hardware investment at ORNL has been in storage capacity (fully operational)
  - 15 PB of disk
  - 30 PB of tape (for redundant backup)

Delivered ahead of schedule and under budget!



The Onyx cluster hosts the ESGF containerized data & index nodes

Data and services reside in the Open Network Enclave of NCCS to provide fast and open access to data

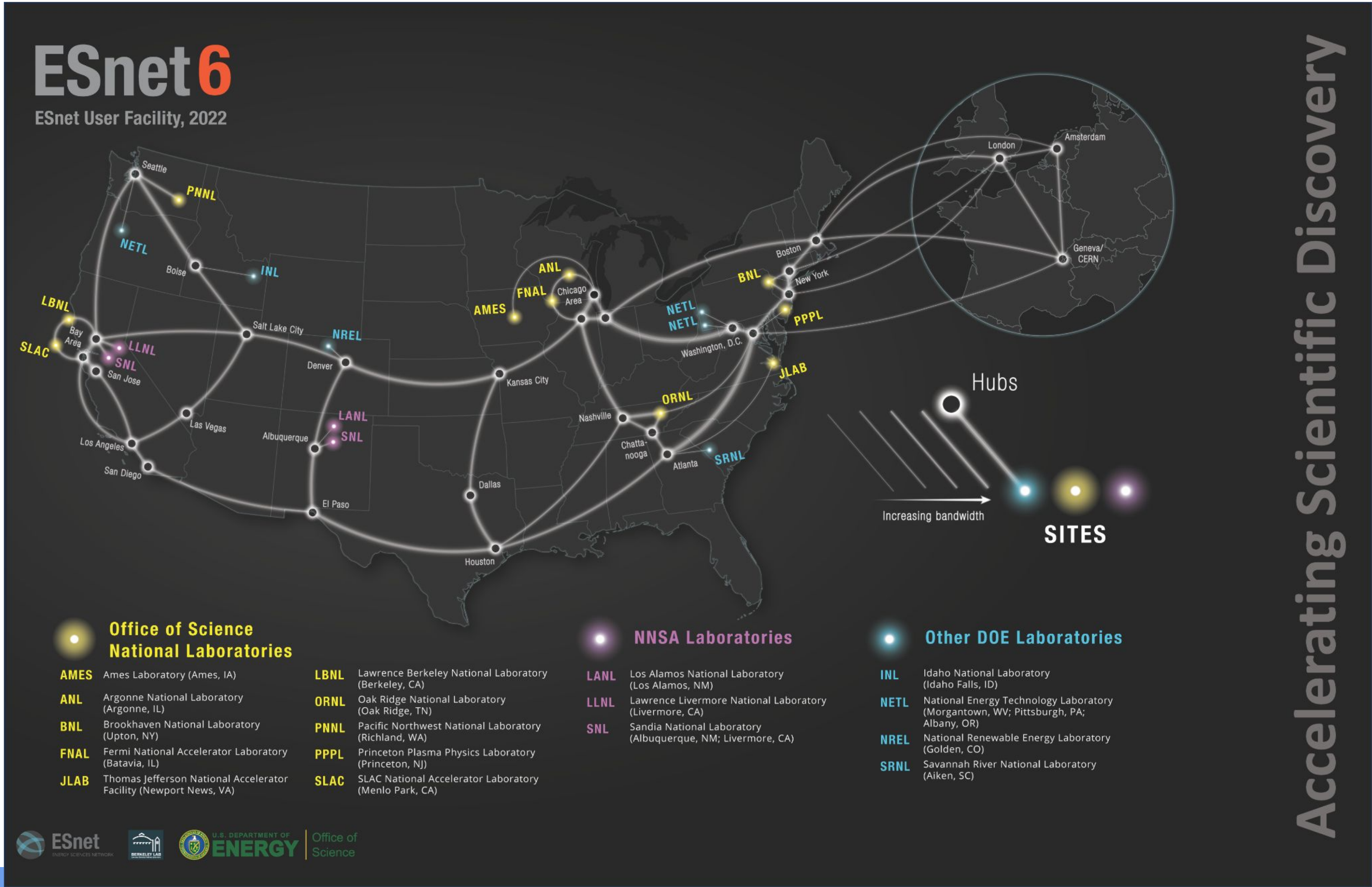
In partnership with the ORNL National Center for Computational Sciences (NCCS)

Expandable tape subsystem of the Themis storage system

ESnet: Fast US Network & Global Connectivity

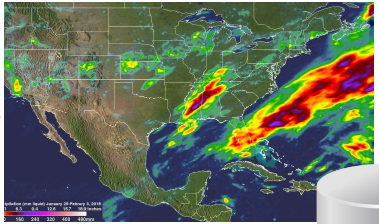
ESGF2-US leverages high bandwidth (100 Gbps) connections to migrate and cache data among DOE Labs, HPC centers, and other institutions.

High speed global interconnectivity enables rapid replication of data across the Federation.



ESGF2 US Enabling a new level of research productivity

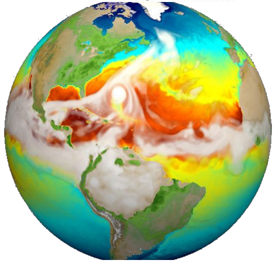
Logging in with her ***institutional credentials****, Samantha is presented with* ***new data, code, and papers*** *relevant to her current research. Intrigued by a new report on extreme precipitation events, she examines a* ***Jupyter notebook*** *that implements the method used. Wondering how this method would work with higher-resolution E3SM data, she* ***quickly locates required datasets and runs the notebook on a subset****. Results are promising, so she* ***shares them with collaborators*** *via ESGF2-US federated storage, and they agree that a larger ensemble analysis is called for. ESGF2-US confirms that the full ensemble data are available at OLCF, so they submit a request to execute the analysis there. Within 24 hours,* ***results have been published to ESGF2-US for broader consumption****, along with the notebook used to produce and validate the results.*



ESGF Earth System Grid Federation

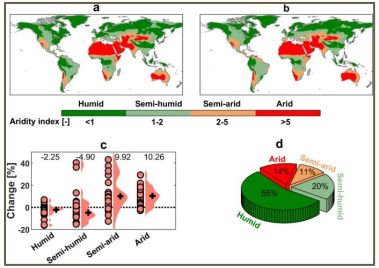
E3SM Energy Exascale Earth System Model

GitHub



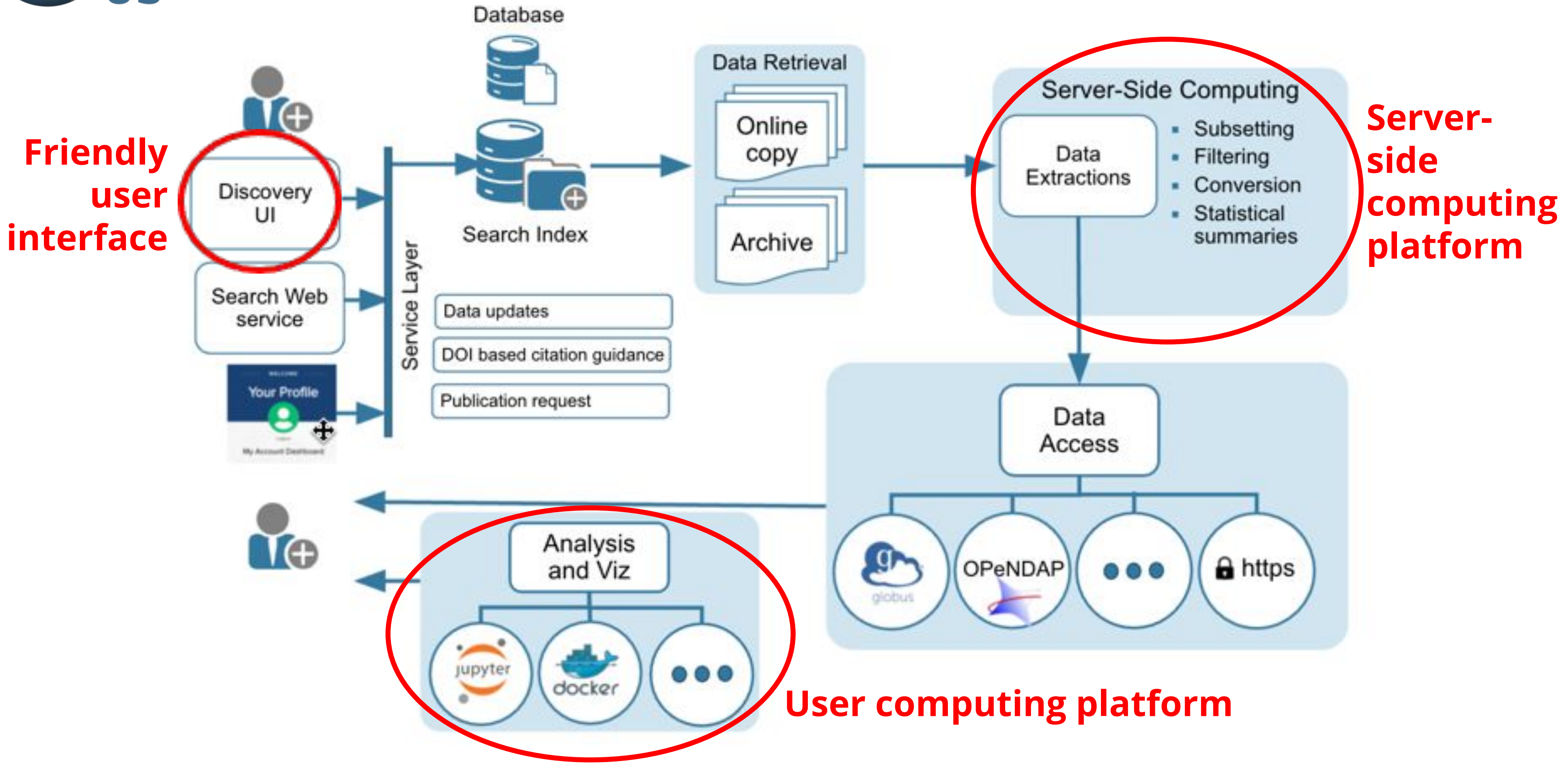
jupyter

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY



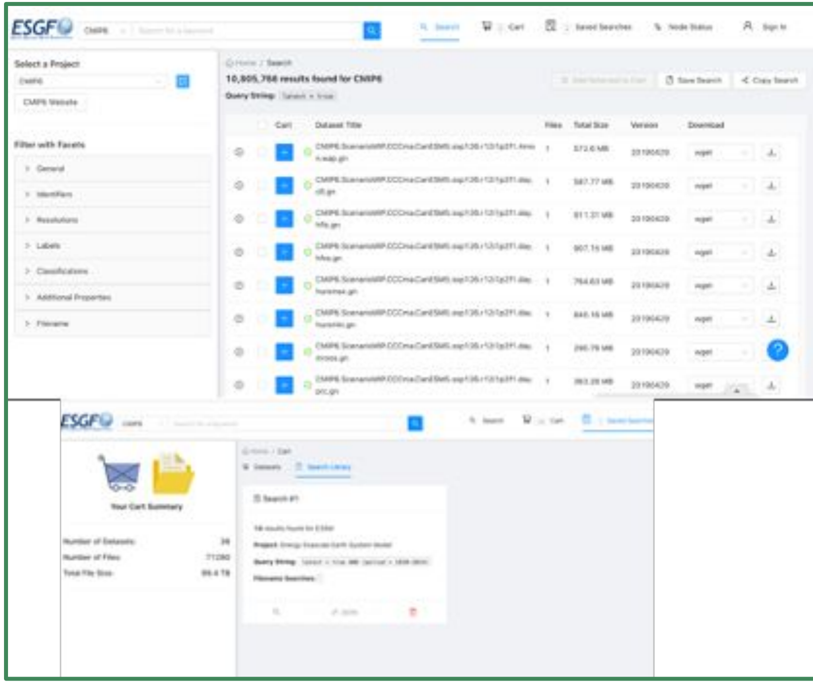
Flood risk increases with rising soil moisture

Data Discovery, Access & Analysis Platform



ESGF2 US Metagrid Enhances ESGF Search

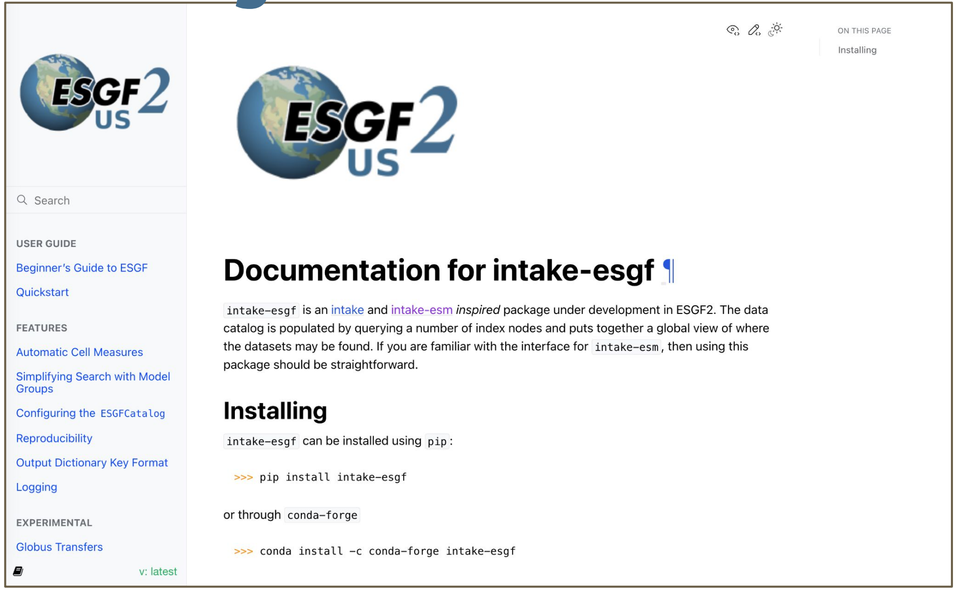
- New **Metagrid faceted search user interface**, developed at LLNL on popular React Javascript framework, deployed at ORNL, LLNL and ANL
- Offers new features, including a **shopping cart**, ability to **save and share searches**, integration with **Globus authentication & transfer** and a search page **tour & support dialog**
- User experience enhancements make it **faster and easier** to discover published data
- **Globus integration** offers faster and more reliable data access
- Will be deployed internationally across the Federation by mid-2024



The Metagrid Web Interface for ESGF search is a completely redesigned interface from CoG. It features a familiar faceted search and a new capability to save searches.

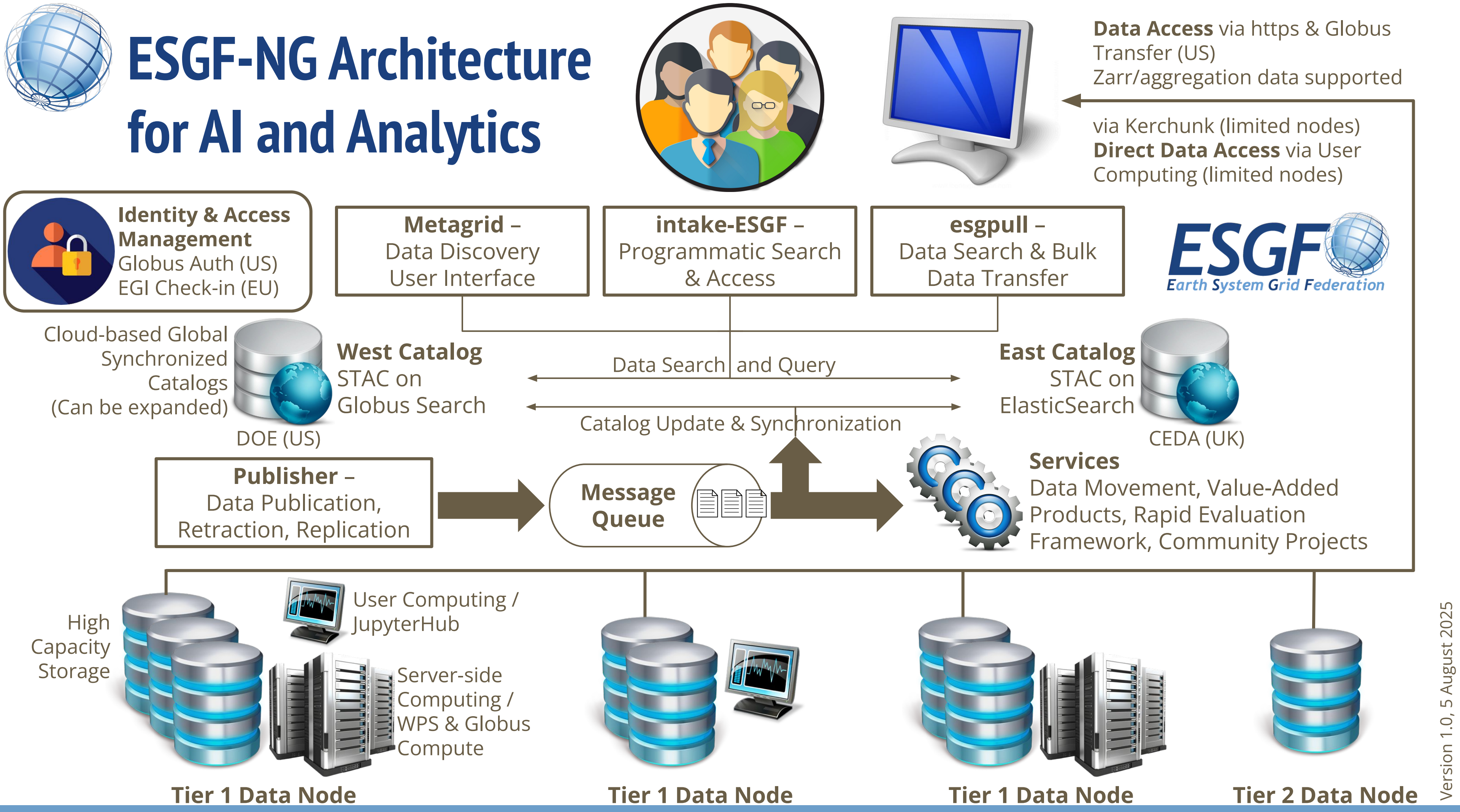
Integrating with intake-esgf

- Improve the APIs to access data; simplify searching for data programmatically across the federation
- Provide STAC-based index query in addition to the existing Solr and Globus indices
- Extend the interface to provide capability for data streaming (OPeN-DAP, Kerchunk, Virtual Zarr) as available
- Integrate the errata service provided by es-doc into intake-esgf catalogs



- Intelligently determines the quickest way to access data (download, Globus Transfer, stream, load locally)
- **Provides method to package compute + flows**

Repository: https://github.com/esgf2-us/intake-esgf
Documentation: https://intake-esgf.readthedocs.io/
Installation: PyPI and Conda-forge

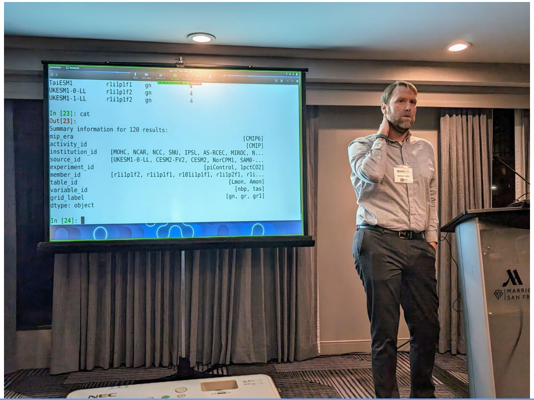

ESGF-NG Architecture for AI and Analytics
Data Access via https & Globus Transfer (US)
Zarr/aggregation data supported
via Kerchunk (limited nodes)
Direct Data Access via User Computing (limited nodes)
Identity & Access Management
Globus Auth (US)
EGI Check-in (EU)
Metagrid – Data Discovery User Interface
intake-ESGF – Programmatic Search & Access
esgpull – Data Search & Bulk Data Transfer
ESGF
Earth System Grid Federation
Cloud-based Global Synchronized Catalogs (Can be expanded)
West Catalog
STAC on Globus Search
DOE (US)
Data Search and Query
Catalog Update & Synchronization
East Catalog
STAC on ElasticSearch
CEDA (UK)
Publisher – Data Publication, Retraction, Replication
Message Queue
Services
Data Movement, Value-Added Products, Rapid Evaluation Framework, Community Projects
High Capacity Storage
User Computing / JupyterHub
Server-side Computing / WPS & Globus Compute
Tier 1 Data Node
Tier 1 Data Node
Tier 1 Data Node
Tier 2 Data Node
Version 1.0, 5 August 2025

ESGF2 US

Outreach Activities

Ninth ESGF Developer and User Conference held jointly between Oak Ridge National Laboratory (USA) and Toulouse (France), January 18–20, 2023

ESGF Workshop & Tutorial at the 2023 AGU Fall Meeting in San Francisco & 2024 AGU Fall Meeting in Washington, DC



ESGF2 US Summary of Integration Activities

- All **ESGF development is being performed collaboratively** with Federation partners
- **User computing** approaches deployed through on-premise infrastructure will enable data-proximate computing
- Specific **integration activities**:
  - **Sharing data indexes** across DOE-BER platforms (ARM Data Center, ESS-DIVE, etc.)
  - Unifying on **Federated authentication** (*Globus Auth*) to simplify data access and enable cross-platform/cross-facility data access and analysis
  - **Integrating software stacks** for data access, analysis, and visualization for Jupyter
  - New global **scalable data indexes** and search instances (*Globus Search*)
  - **Managed automation** of data publishing workflows (*Globus Flows*)
  - **Server-side computing** spawned by web or Jupyter/Python (*Web Processing Service* and *Globus Compute*) for generating value-added products and subsetting & summarizing data across platforms and facilities
- New technologies might enable (1) *streaming data into HPC for AI training*, (2) *dynamic job scheduling and migration*, and (3) *generation of value-added products "on the fly"*

Questions?