U.S. DEPARTMENT OF ENERGY
Office of Science

Exploiting Artificial Intelligence and Machine Learning for Advancing Earth System Prediction

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COEAI-SPARC Workshop on Hybrid Physics-AI Models for Climate, Weather and Water

June 19–21, 2024 at Maitreyee Auditorium, IIT Kharagpur, India

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 #1 fastest supercomputer on the [TOP500](TOP500) List (May 13, 2024) and the first supercomputer to break the exaflop barrier (May 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/

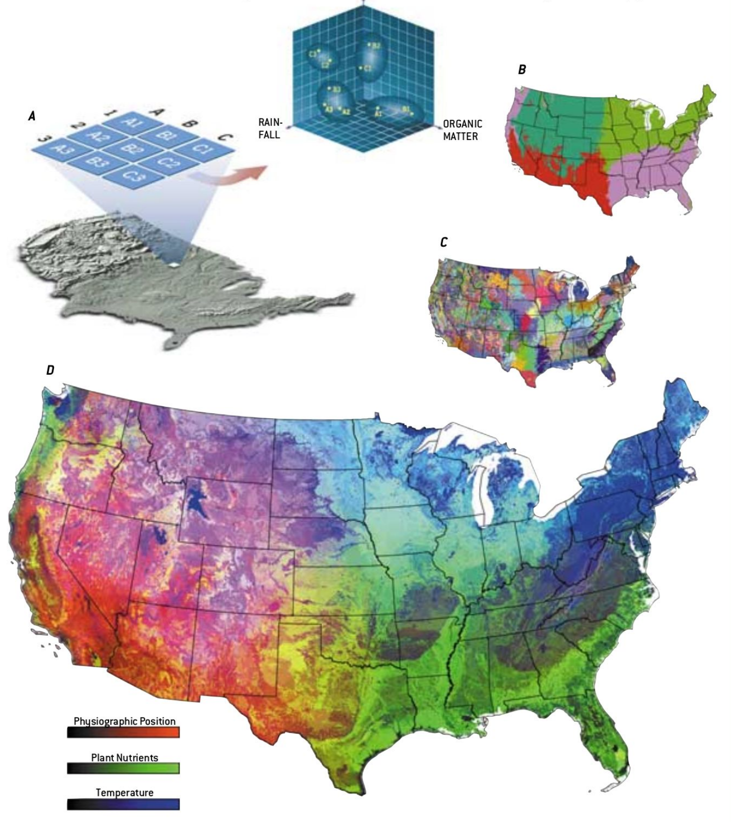
Multivariate Geographic Clustering

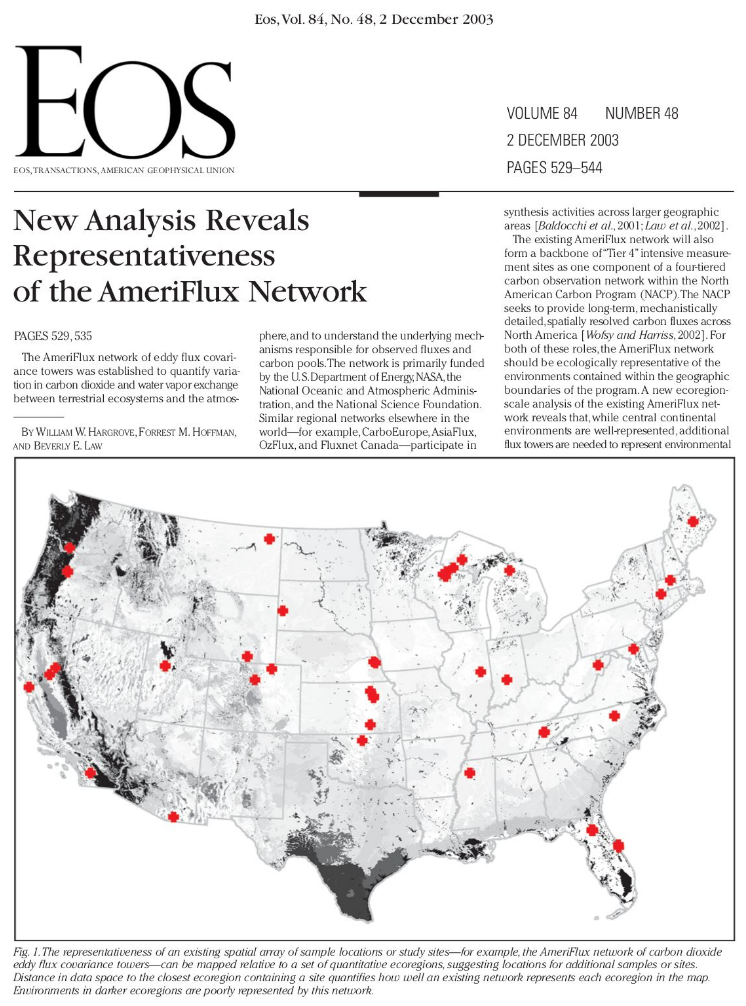
- Ecoregions have traditionally been created by experts
- Our approach has been to objectively create ecoregions using continuous continental-scale data and clustering
- We developed a highly scalable *k*-means cluster analysis code that uses distributed memory parallelism
- Originally developed on a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

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/

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 ecoregions provides far more detail (*C*). Another approach is to represent three composite characteristics with varying levels of red, green and blue (*D*).




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.

Network Representativeness

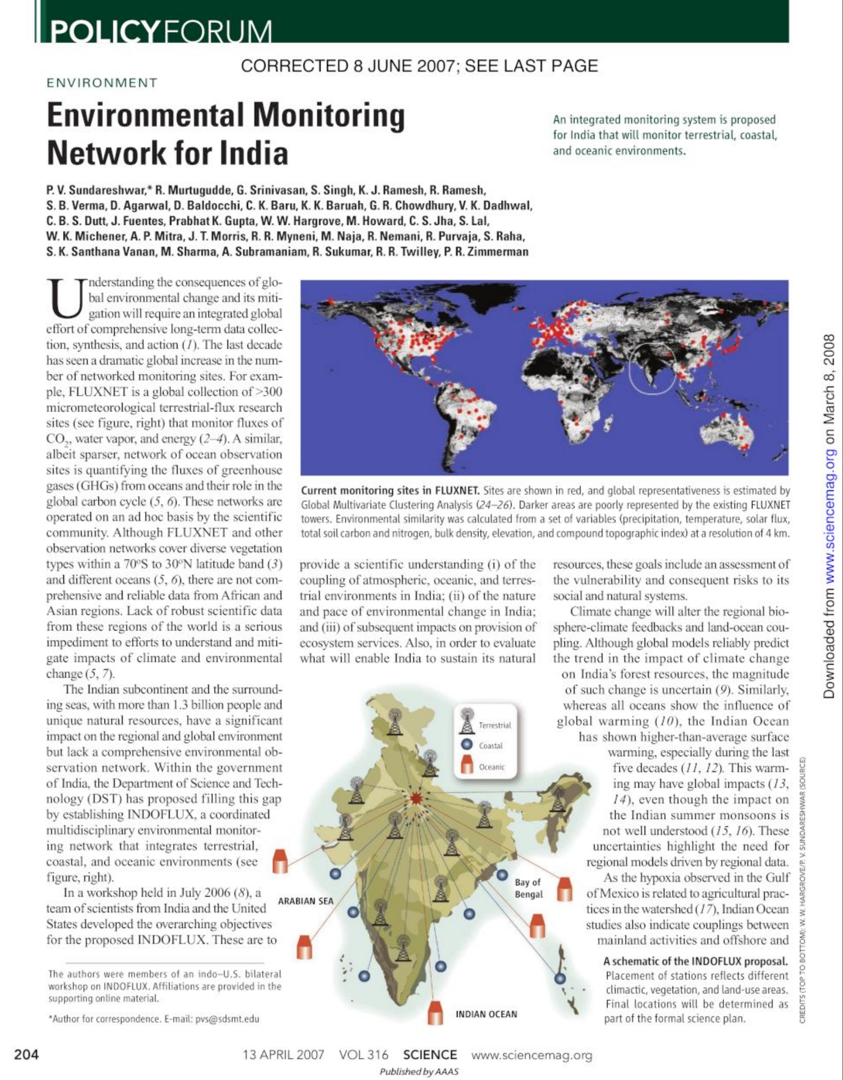
- The *n*-dimensional space formed by the data layers offers a natural framework for estimating representativeness of individual sampling sites
- The Euclidean distance between individual sites in data space is a metric of similarity or dissimilarity
- Representativeness across multiple sampling sites 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).



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.

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

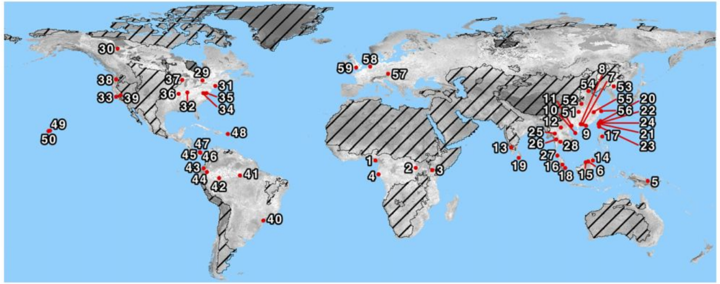


Fig. 1 Map of the CTFS-ForestGEO network illustrating its representation of bioclimatic, edaphic, and topographic conditions globally. Site numbers correspond to ID# in Table 2. Shading indicates how well the network of sites represents the suite of environmental factors included in the analysis; light-colored 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

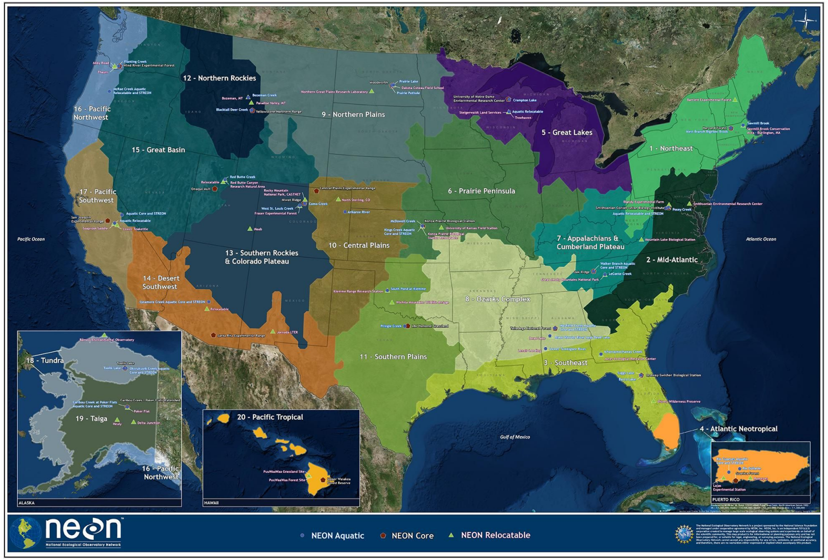
Attribute	Utility
Very large plot size	Resolve community and population dynamics of highly diverse forests with many rare species with sufficient sample sizes (Losos & Leigh, 2004; Condit *et al.*, 2006); quantify spatial patterns at multiple scales (Condit *et al.*, 2000; Wiegand *et al.*, 2007a,b; 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

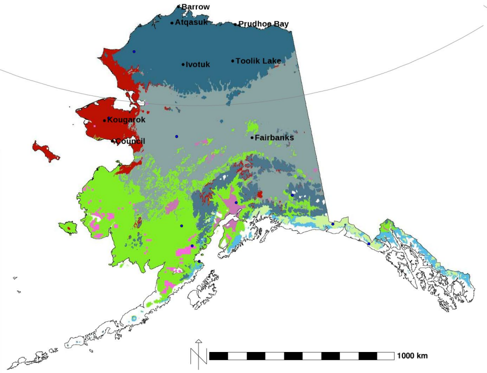
- The CTFS-ForestGEO global forest monitoring network is aimed at characterizing forest responses to global change
- The figure at left shows the global representativeness of the CTFS-ForestGEO sites in 2014
- Non-forested areas are masked with hatching, and as expected, they are consistently darker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

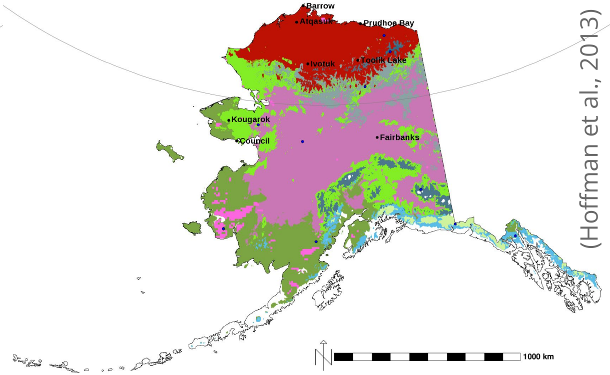
Sampling Network Design



NSF's NEON Sampling Domains



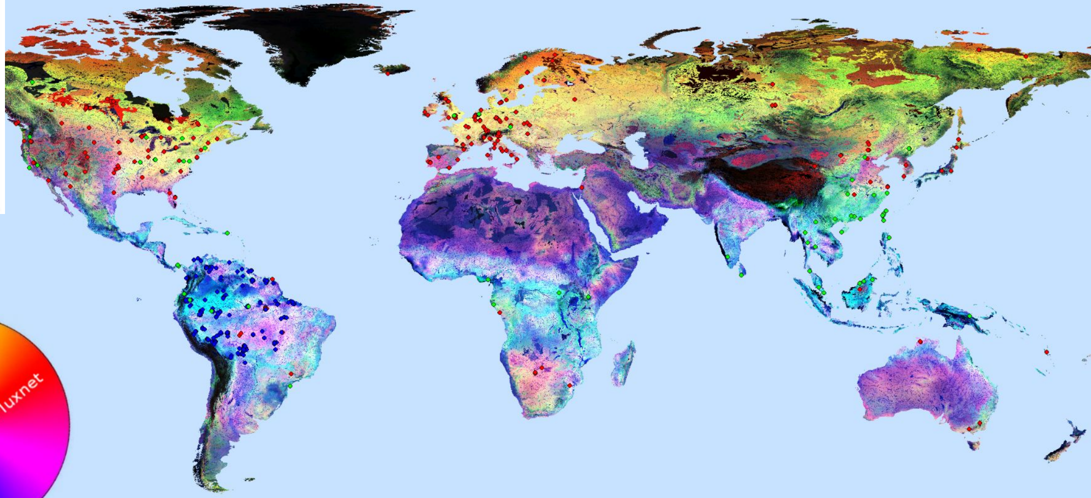
2000–2009

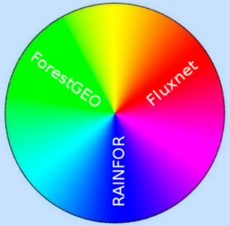


2090–2000

(Hoffman et al., 2013)

Triple-Network Global Representativeness



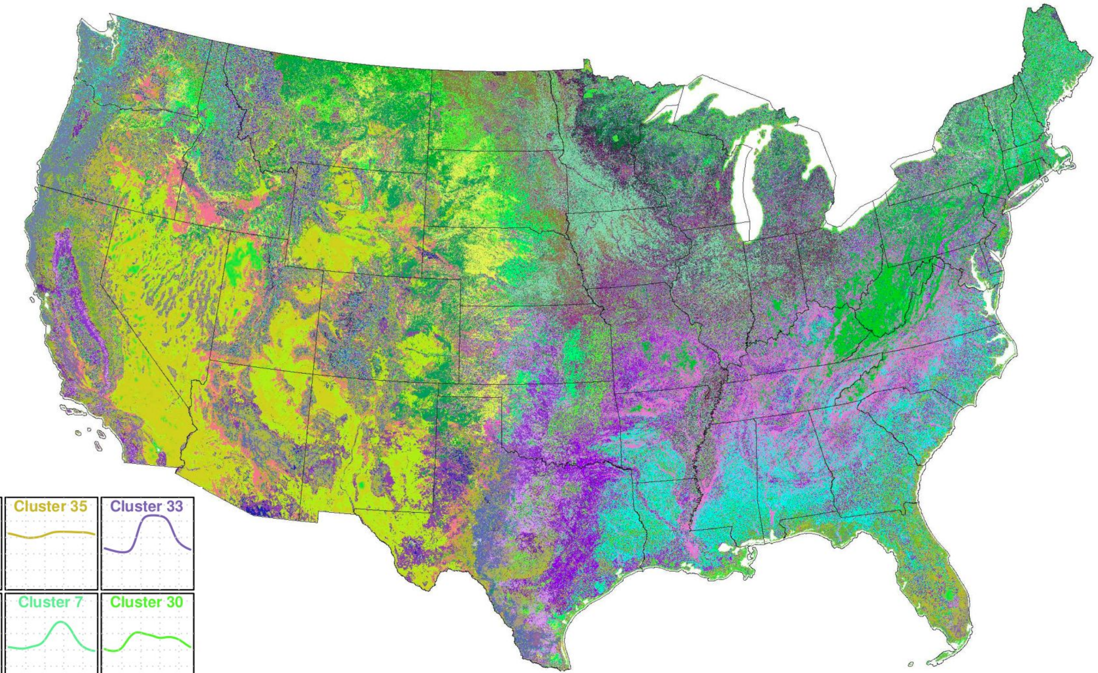


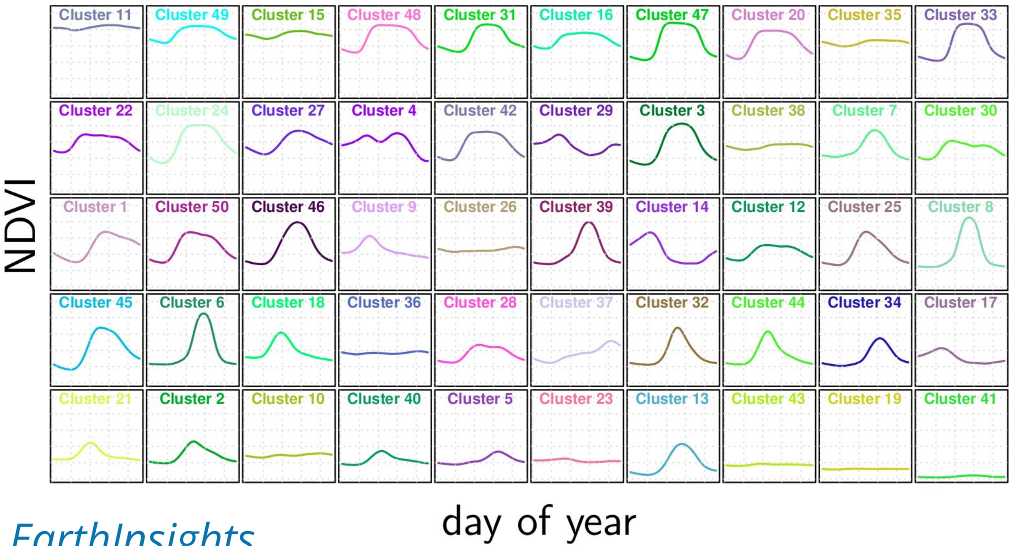
Gridded data from satellite and airborne remote sensing, models, and synthesis products can be combined to design optimal sampling networks and understand representativeness as it evolves through time

(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



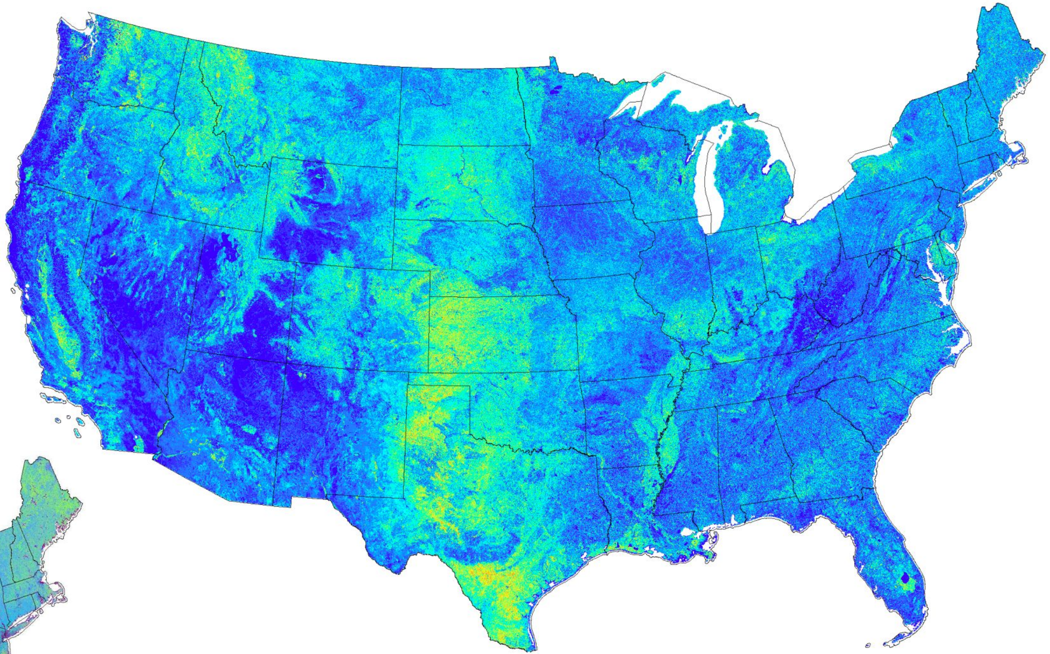


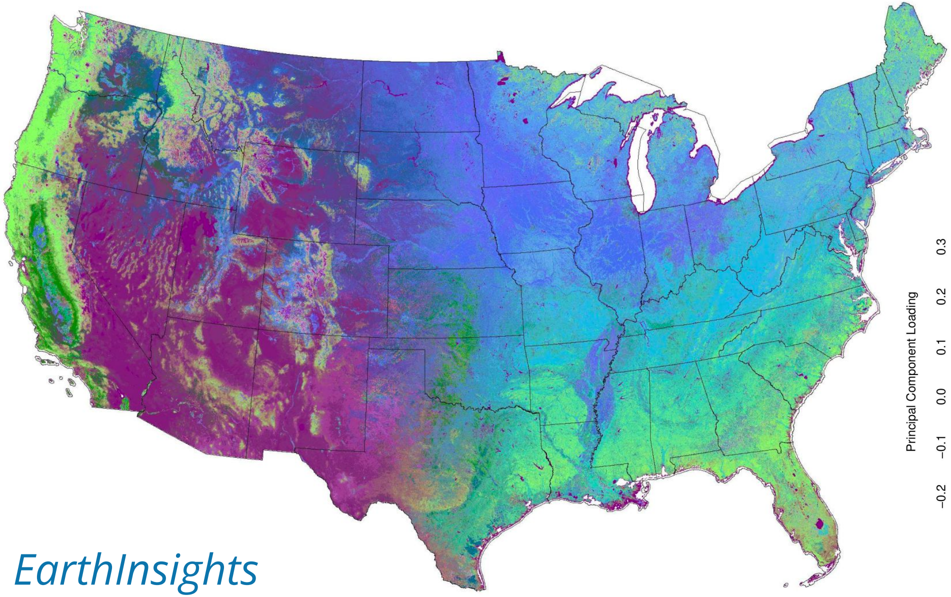
50 Phenoregion Prototypes (Random Colors)

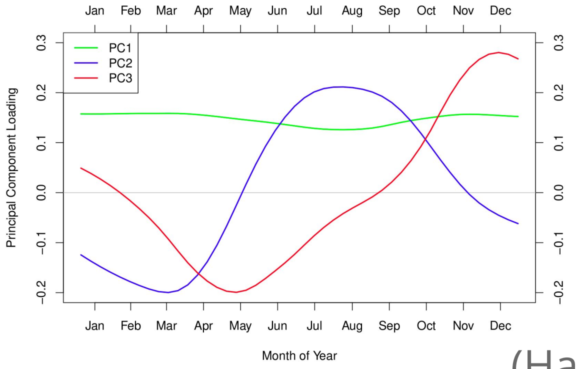
EarthInsights

(Hargrove et al., in prep.)

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







Principal Components Analysis

PC1 ~ Evergreen

PC2 ~ Deciduous

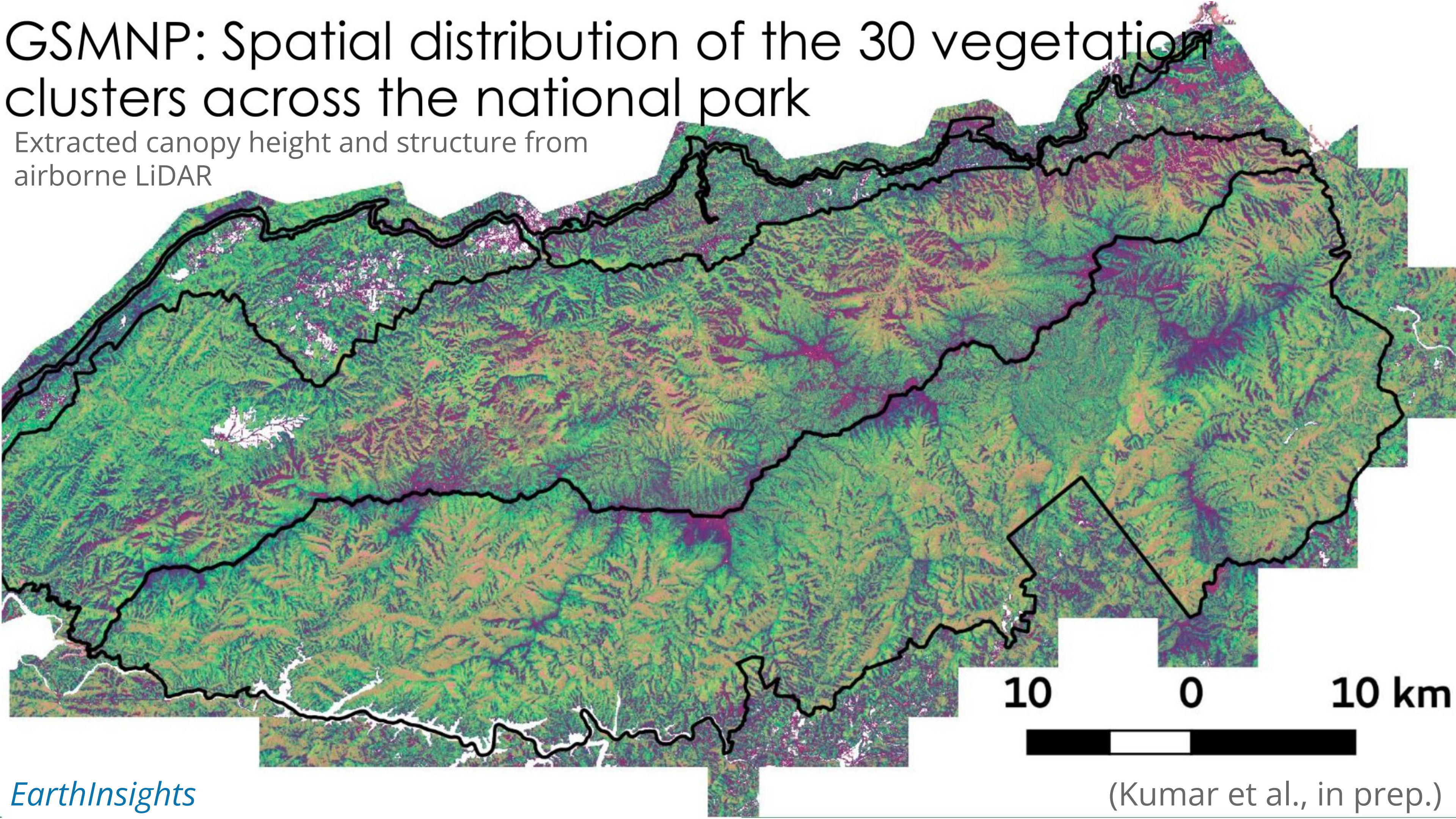
PC3 ~ Dry Deciduous

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



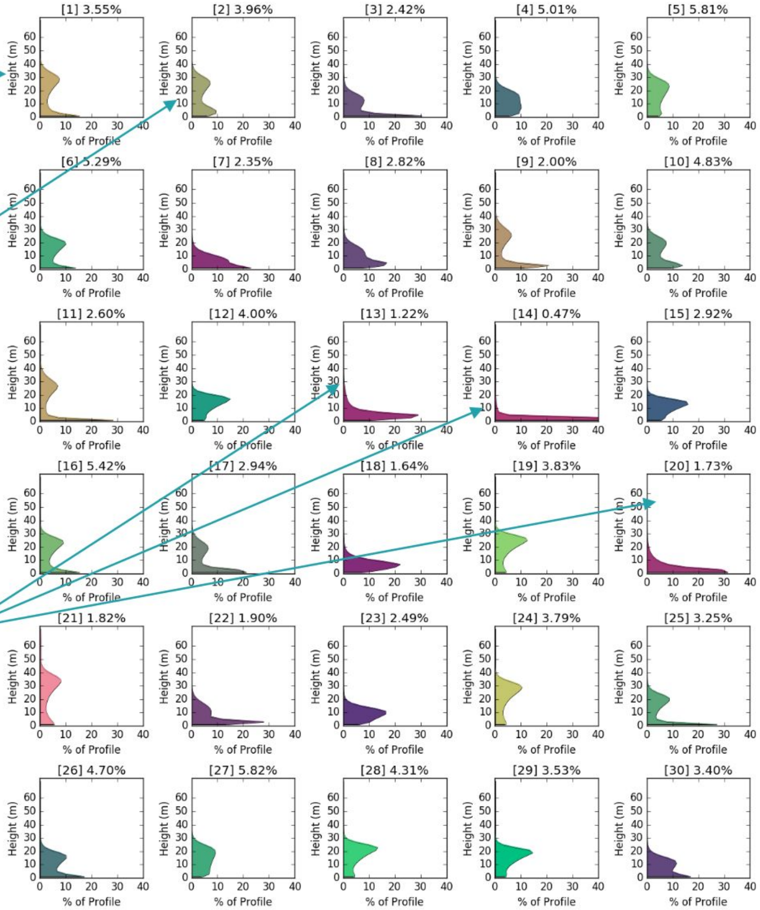
(Kumar et al., in prep.)

GSMNP: 30 representative vertical structures (cluster centroids) identified

tall forests with low understory vegetation

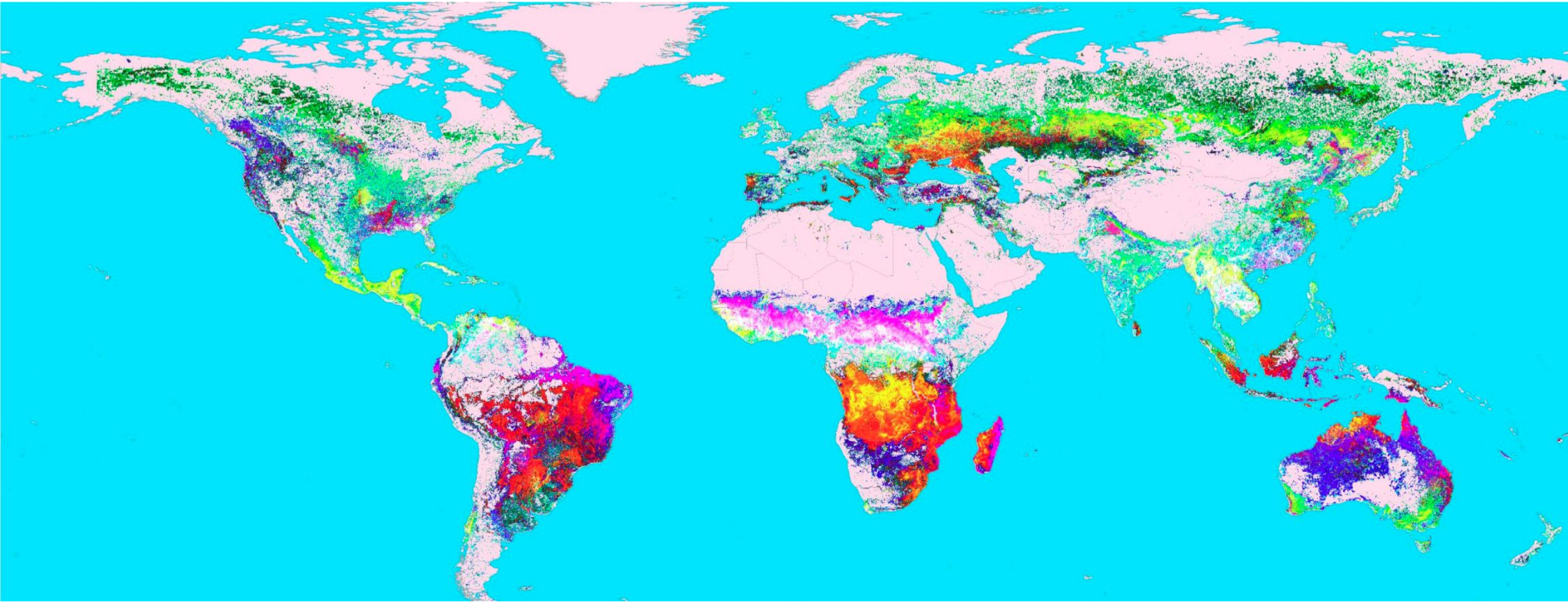
forests with slightly lower mean height with dense understory vegetation

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



(Kumar et al., in prep.)

Global Fire Regimes

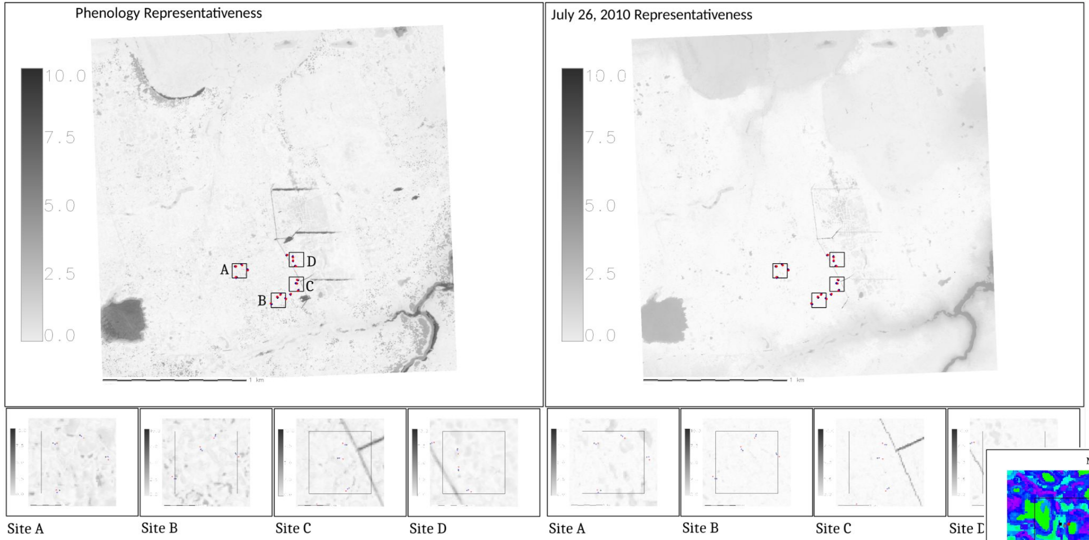


Regions that exhibit similar fire seasonality globally

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

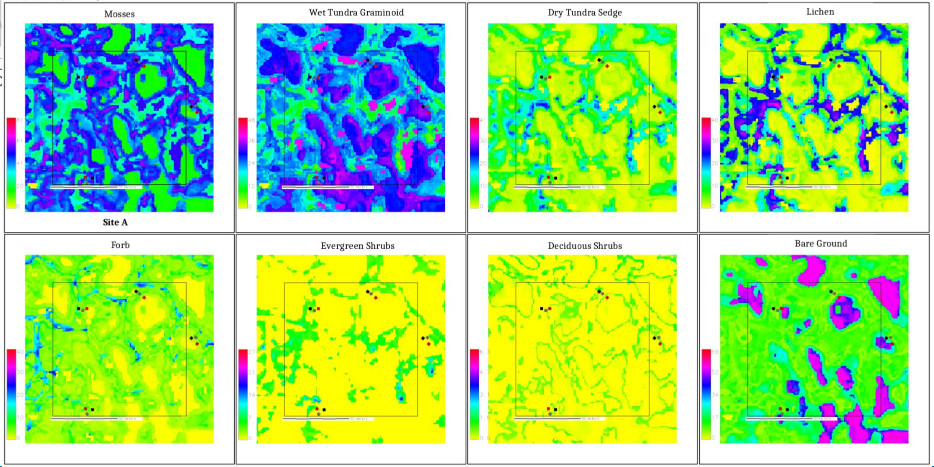
(Norman et al., submitted)

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

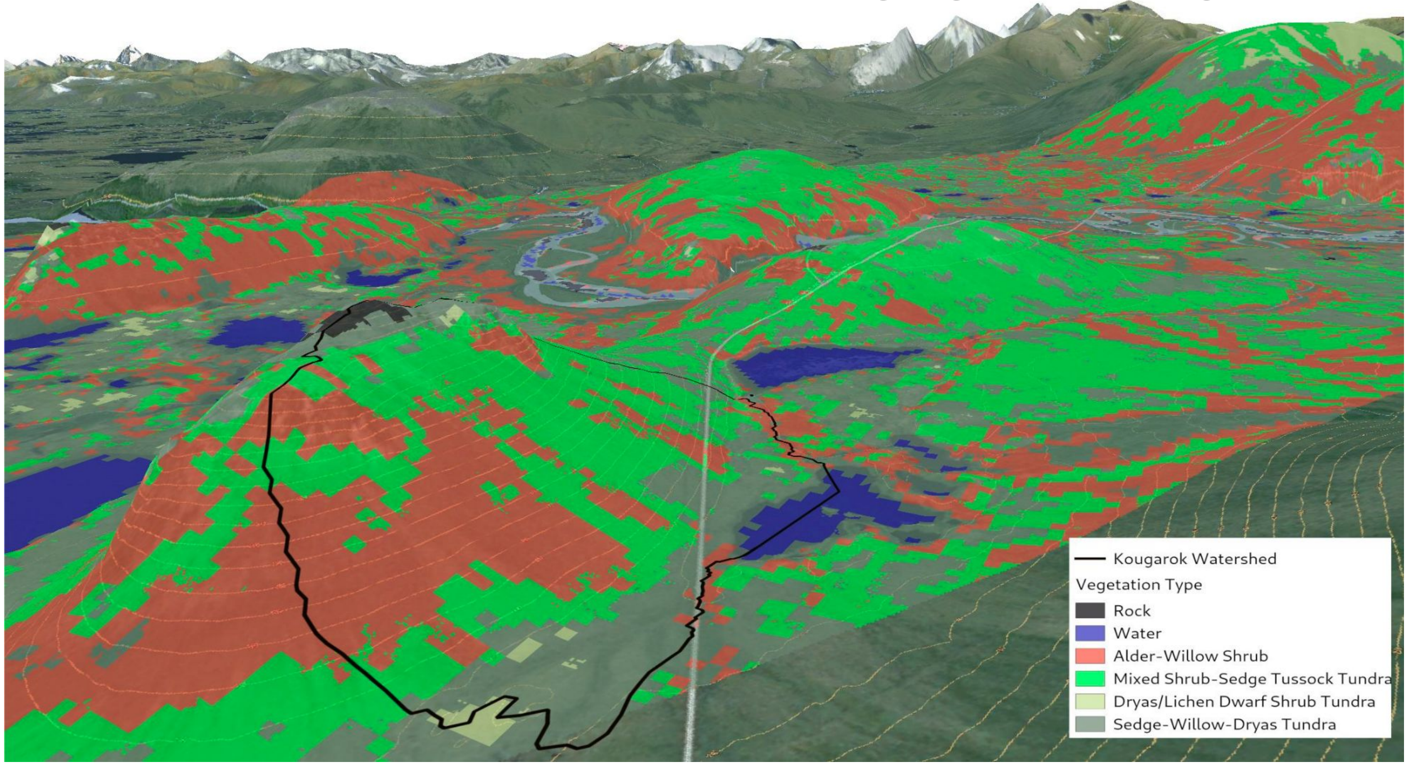


In situ data from field measurement activities inform the development of wide-scale maps of vegetation distribution through inference using remote sensing data as surrogate variables, and relationships with environmental controls can be extracted

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](https://doi.org/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

a)

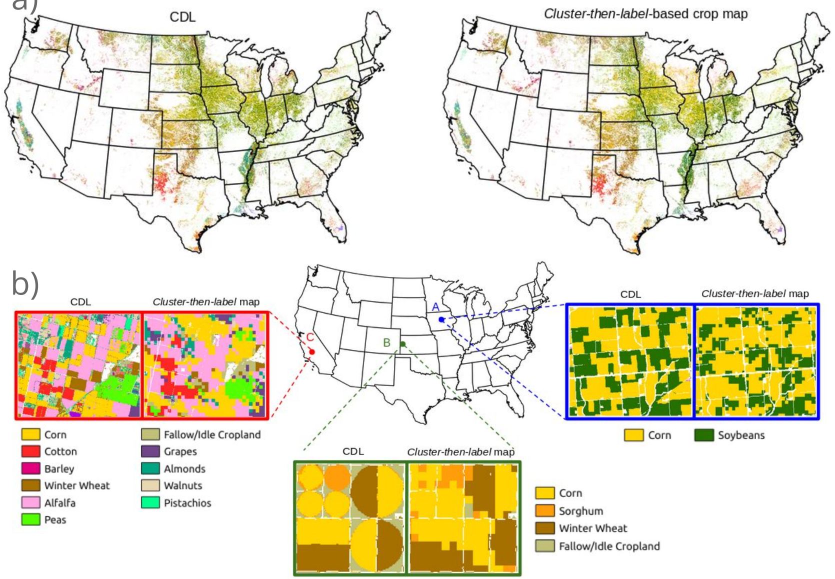
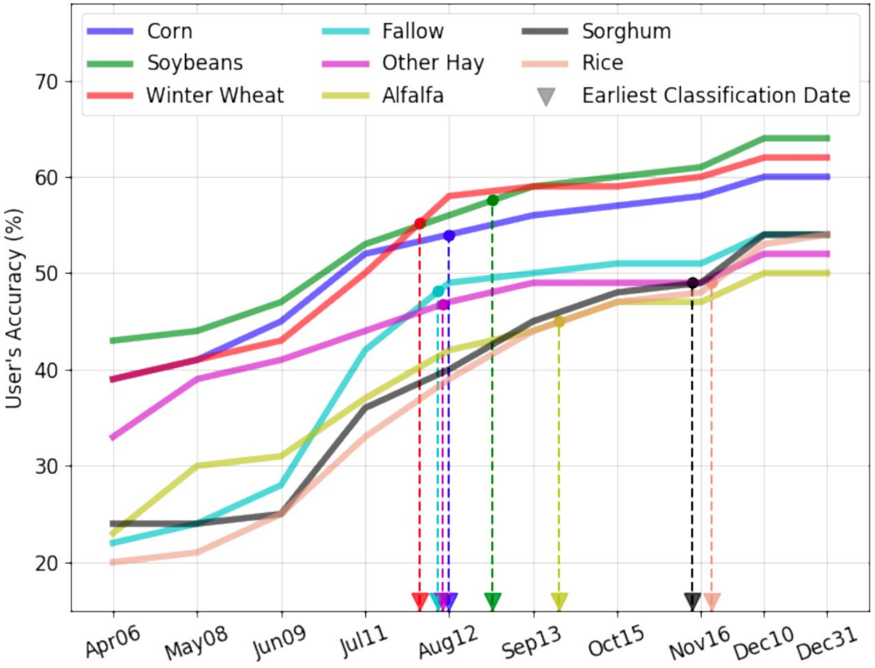


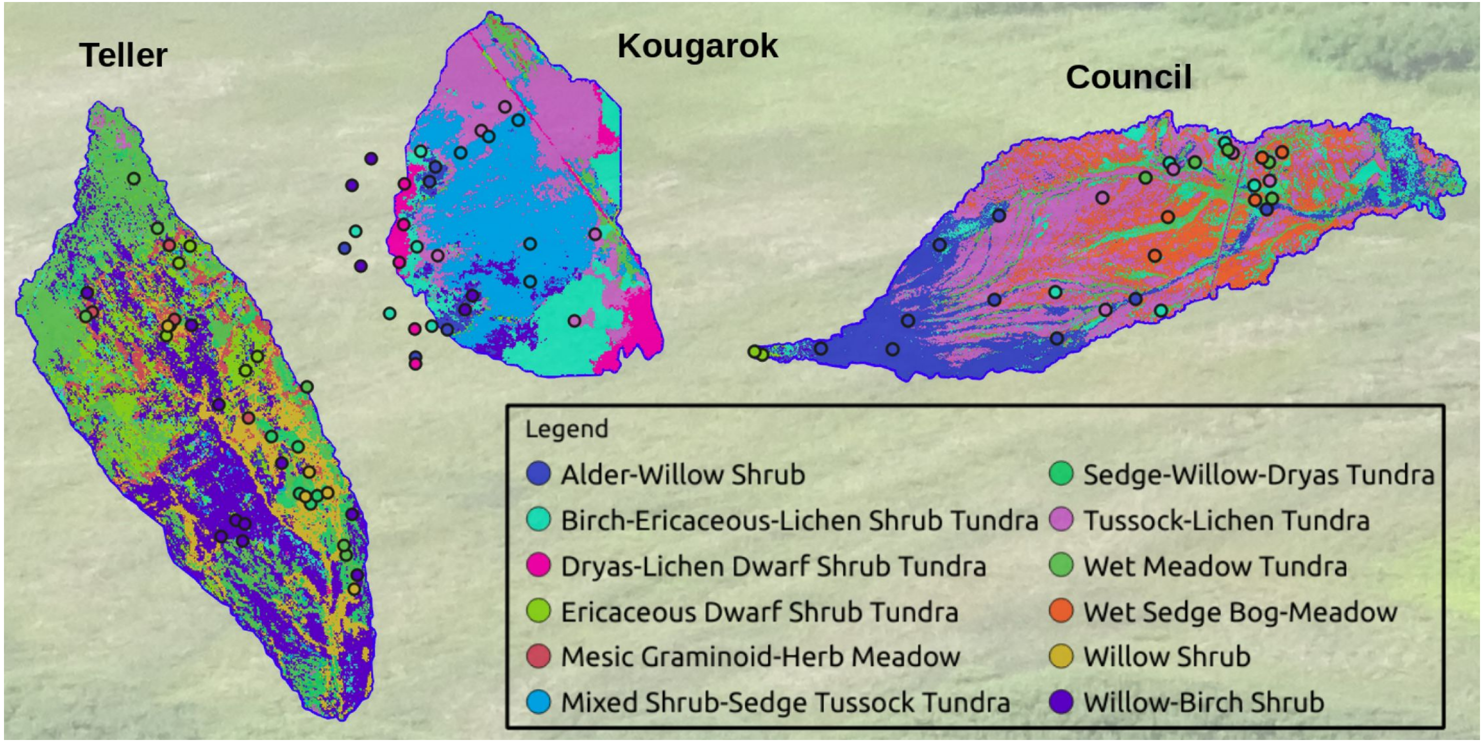
Figure: a) Comparison of cluster-then-label crop map with USDA Crop Data Layer (CDL) shows similar patterns at continental scale. b) Good spatial agreement is found at three selected regions, but cluster-then-label crop maps lack sharpness at field boundaries due to coarser resolution of MODIS data.

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

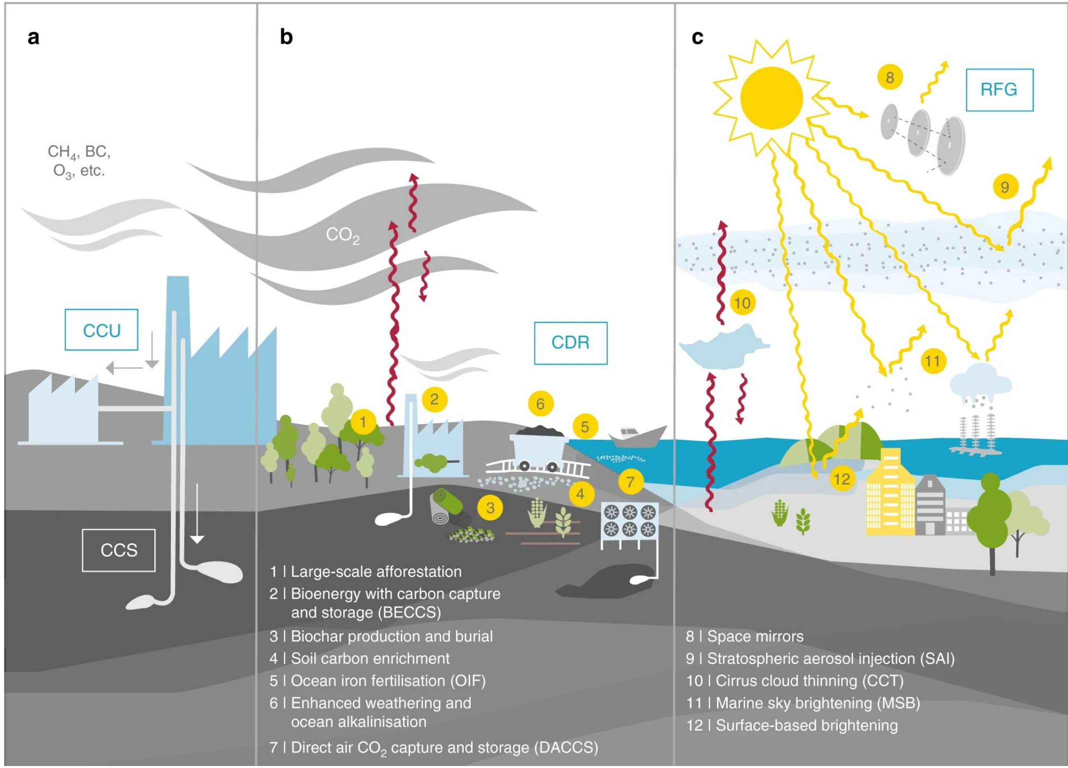


At the watershed scale, vegetation community distribution follows topographic and water controls.
At a fine scale, nutrients limit the distribution of vegetation types.

(Konduri et al., in prep.)

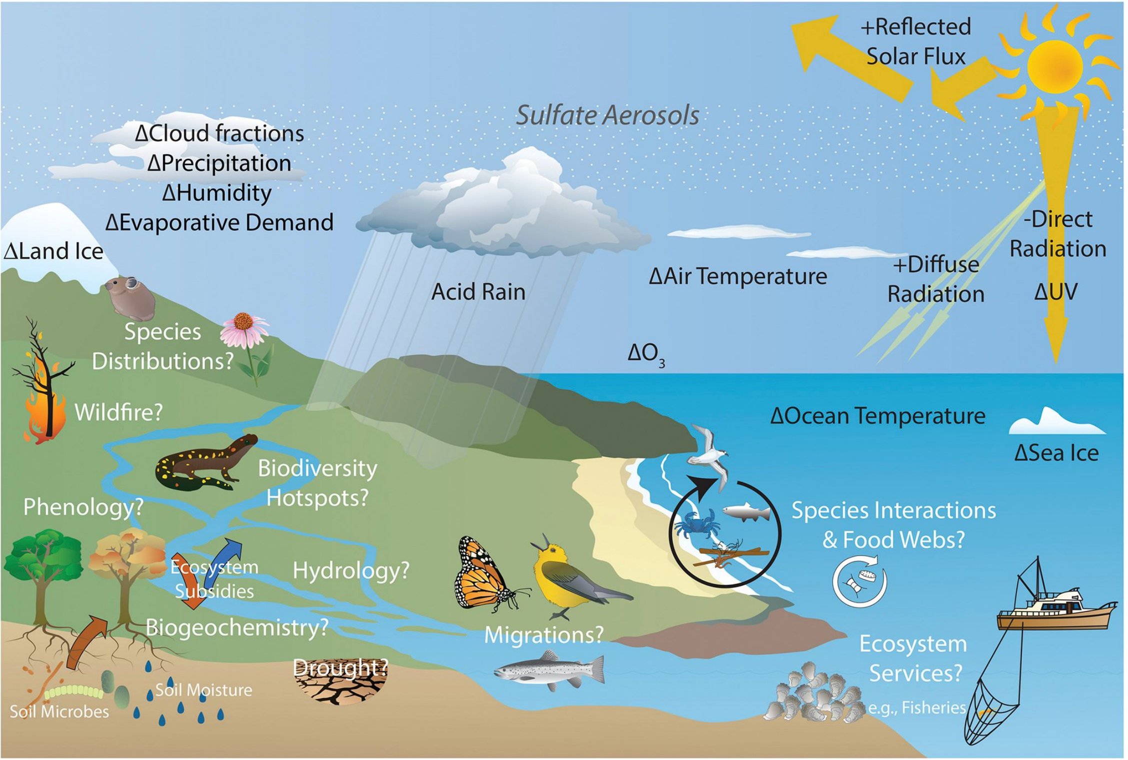
Climate Change Mitigation through Climate Intervention

- The increasing severity of extreme events and wildfire is threatening utilities, built infrastructure, and economic & national security
- Loss of life and property is motivating consideration of *climate intervention* or *geoengineering*
- In addition to *carbon dioxide removal (CDR)* through *direct air capture (DAC)* and other means, interest is growing in reducing or stabilizing Earth's surface temperature
- *Solar radiation management (SRM)* is an approach to partially reduce warming, and *stratospheric aerosol intervention (SAI)* by injecting sulfur into the lower stratosphere is considered the most feasible scheme



A wide variety of natural solutions and geoengineering techniques are proposed for mitigating the effects of climate change. Adopted from Lawrence et al. (2018).

Potential Ecological Impacts of Climate Intervention



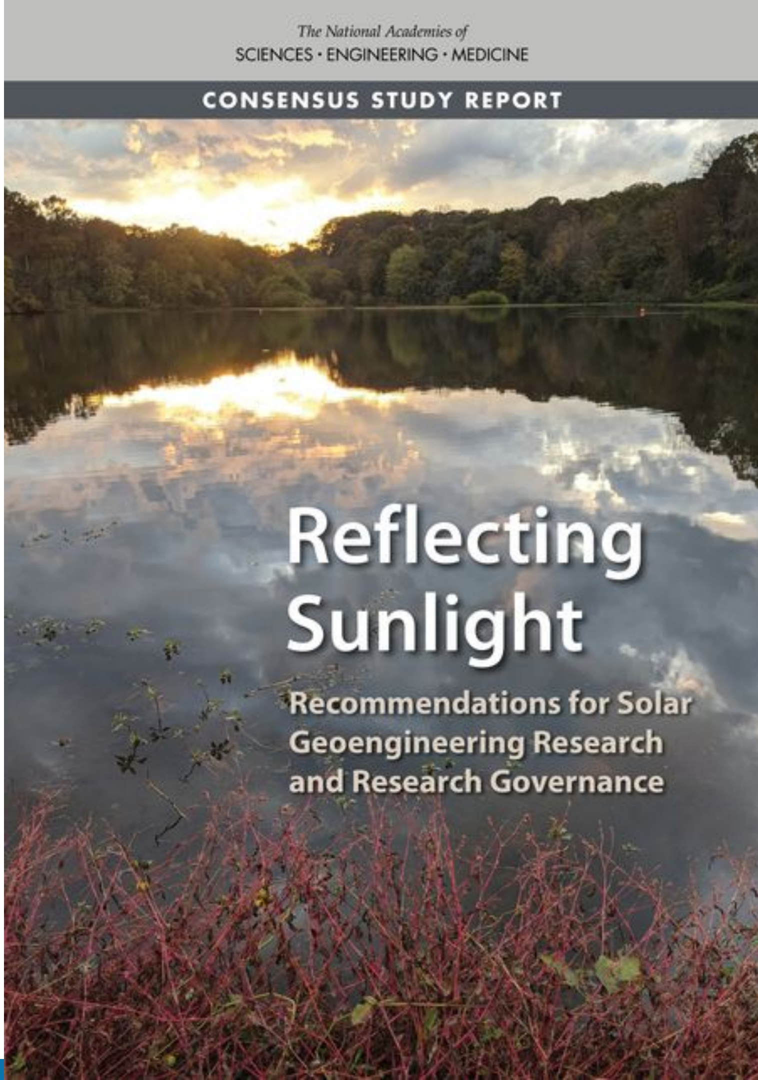
Although some effects of SRM with SAI on climate are known from certain SAI scenarios, the effects of SAI on ecological systems are largely unknown. Adopted from Zarnetske et al. (2021).

- While climate research has focused on predicted climate effects of SRM, few studies have investigated impacts that SRM would have on ecological systems
- Impacts and risks posed by SRM would vary by implementation scenario, anthropogenic climate effects, geographic region, and by ecosystem, community, population, and organism
- A transdisciplinary approach is essential, and **new modeling paradigms are required**, to represent complex interactions across Earth system components, scales, and ecological systems

Climate Intervention Research

A 2021 report from the National Academies of Sciences, Engineering, and Medicine (NASEM) concludes **a strategic investment in research is needed** to advance policymakers' understanding of climate response options.

> *The US should develop a transdisciplinary research program, in collaboration with other nations, to advance understanding of solar geoengineering's technical feasibility and effectiveness, possible impacts on society and the environment, and social dimensions such as public perceptions, political and economic dynamics, and ethical and equity considerations.*



Geoengineering Increases the Global Land Carbon Sink

Objective: To examine stratospheric aerosol intervention (SAI) impacts on plant productivity and terrestrial biogeochemistry.

Approach: Analyze and compare simulation results from the Stratospheric Aerosol Geoengineering Large Ensemble (GLENS) project from 2010 to 2097 under RCP8.5 with and without SAI.

Results/Impacts: In this scenario, SAI causes terrestrial ecosystems to store an additional 79 Pg C globally as a result of lower ecosystem respiration and diminished disturbance effects by the end of the 21st century, yielding as much as a 4% reduction in atmospheric CO_2 mole fraction that progressively reduces the SAI effort required to stabilize surface temperature.

Yang, C.-E., **F. M. Hoffman**, D. M. Ricciuto, S. Tilmes, L. Xia, D. G. MacMartin, B. Kravitz, J. H. Richter, M. Mills, and J. S. Fu (2020), Assessing Terrestrial Biogeochemical Feedbacks in a Strategically Geoengineered Climate, *Environ. Res. Lett.*, doi:10.1088/1748-9326/abacf7.

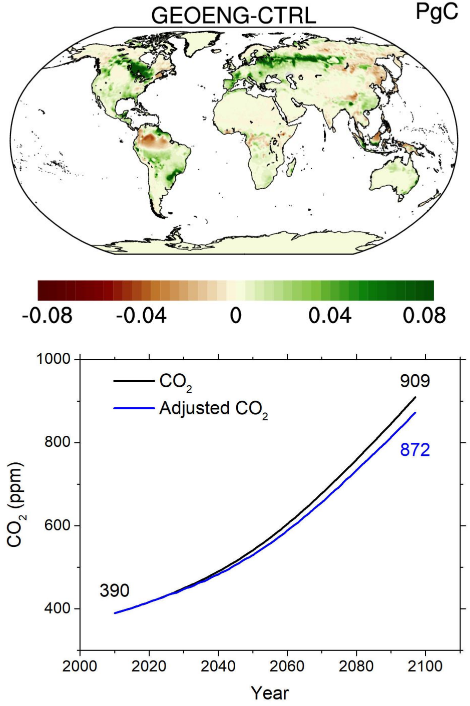
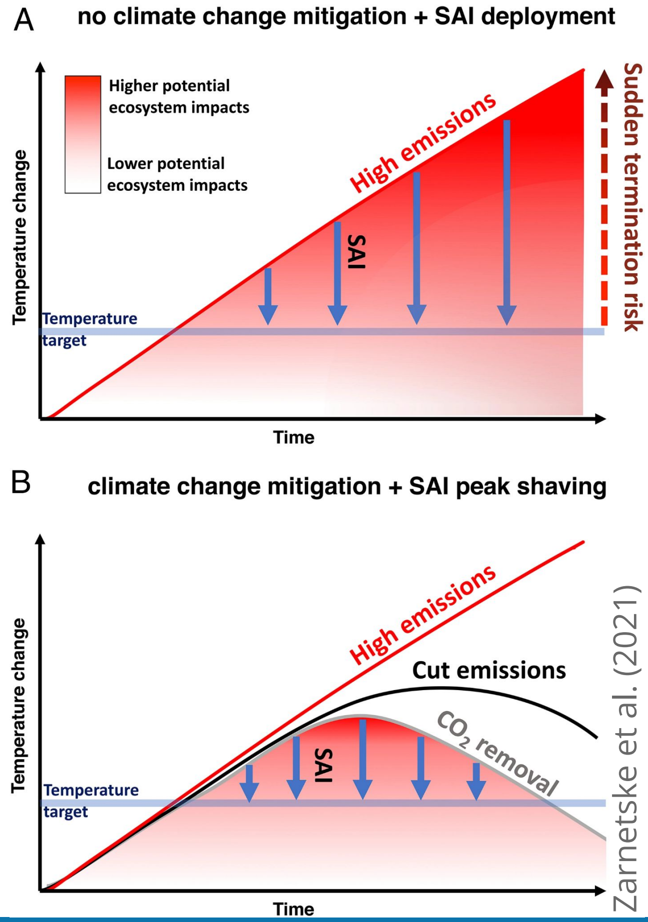


Figure: The larger sink under SAI increased land C storage by 79 Pg C by 2097, which would reduce the projected atmospheric CO_2 level.

Exploring Feedbacks of SAI

- To fill research gaps in understanding Earth system feedbacks of SAI on ecosystems, we are conducting a series of increasingly complex geoengineering simulations with **DOE's Energy Exascale Earth System Model (E3SM)**
- **Simulations will mimic effects of CDR, SAI, and CDR plus SAI**
- Start with SSP5-3.4-OS mid-range overshoot CO_2 trajectory from CMIP6, which prescribes a drawdown of CO_2
- Global surface temperatures will rise by >2.5°C around 2040, **above the 2°C threshold that may induce irreversible impacts**
- Next, introduce SAI to simultaneously cool the surface until drawdown is sufficient to assure < 2°C warming, called **temperature "peak shaving"**
- To quantify feedbacks from reducing, not increasing, atmospheric CO_2, **but may not capture all the as yet unobserved processes**



Zarnetske et al. (2021)

Leveraging Advances in Machine Learning for Earth Sciences

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

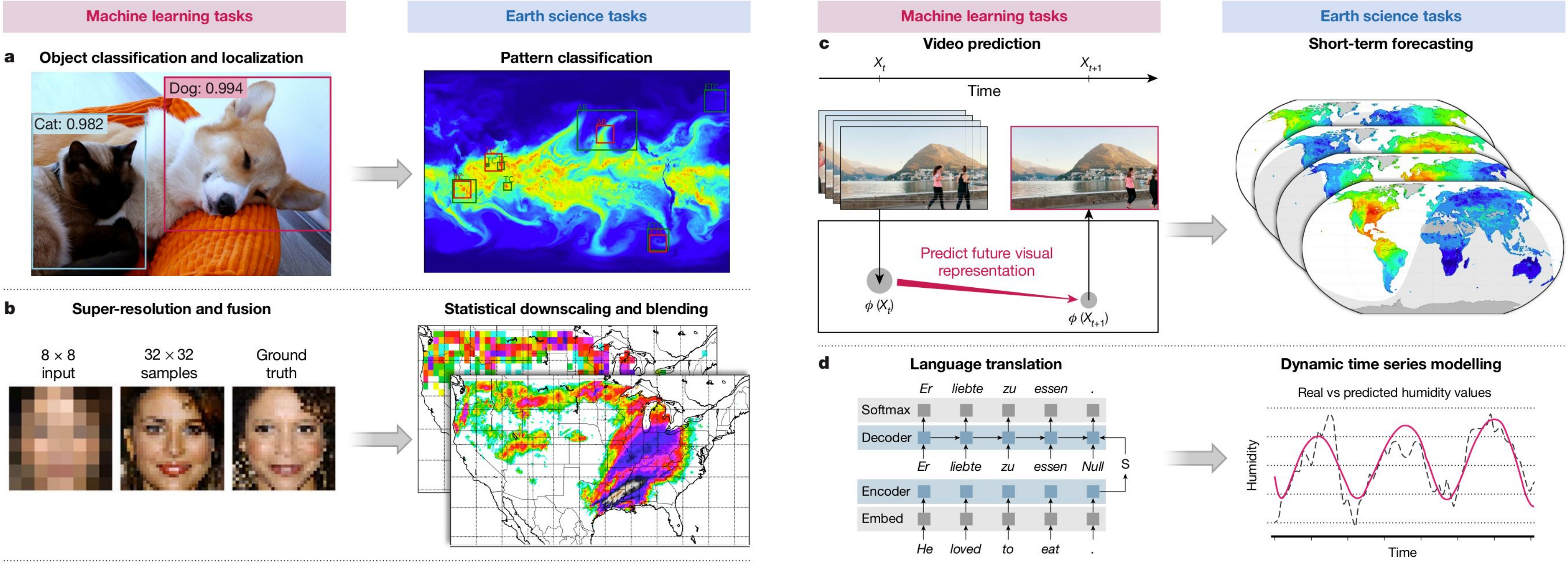
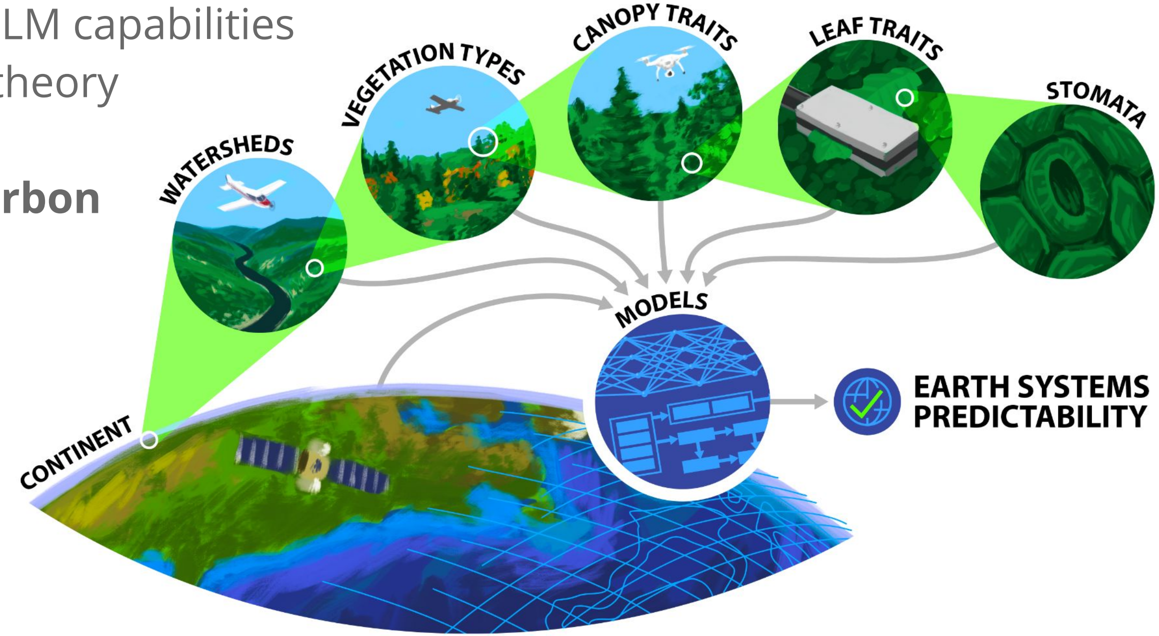


Figure 2 in Reichstein et al. (2019)

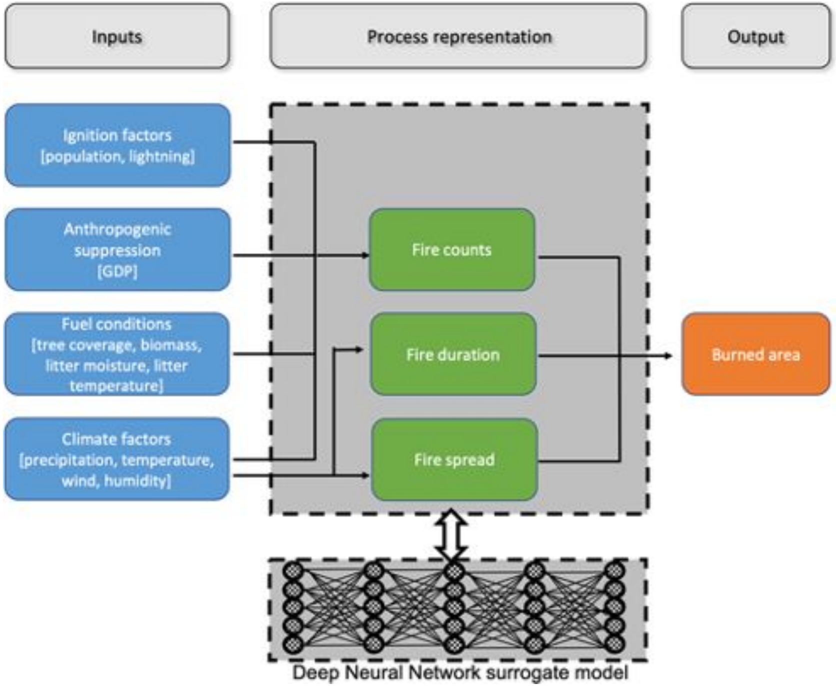
Machine Learning for Understanding Biospheric Processes

- 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

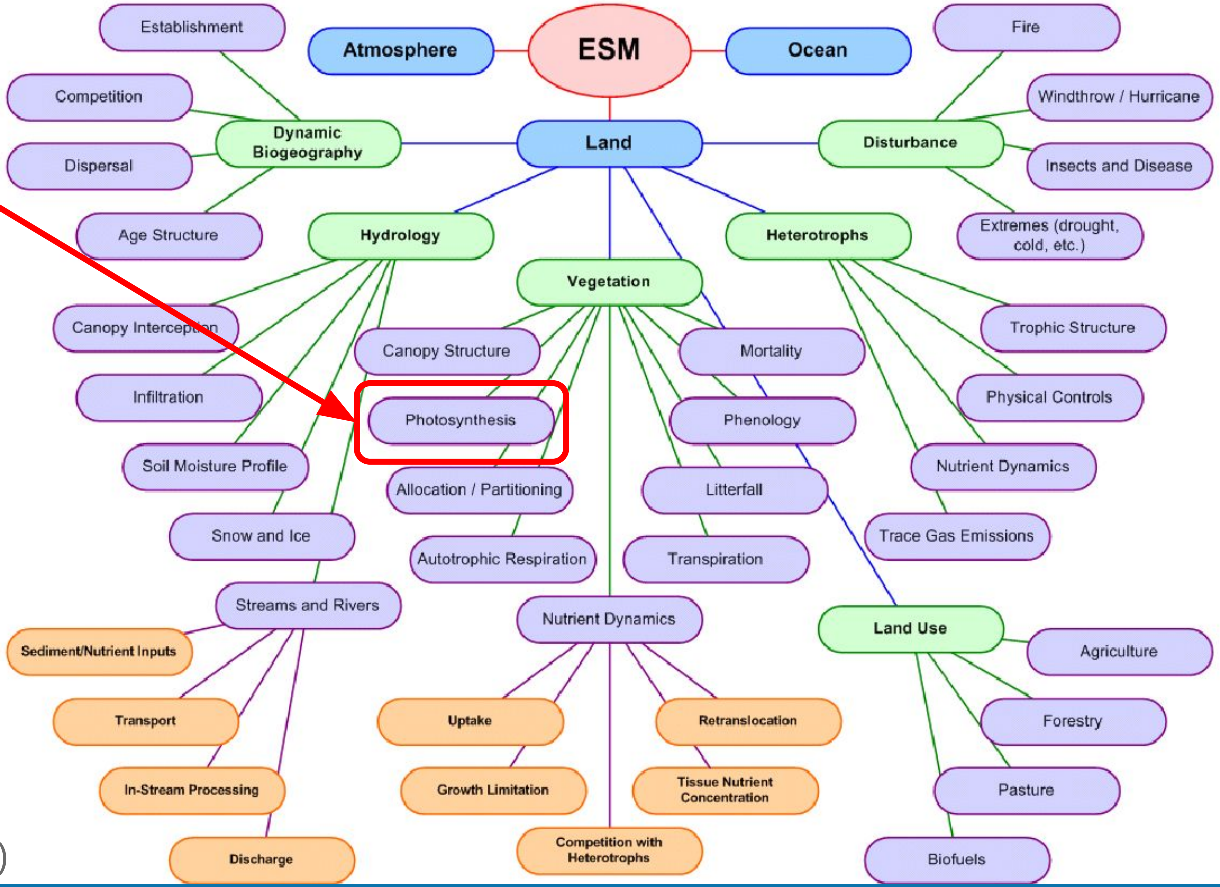


Zhu et al. (2022)

Hybrid ML/Process-based Modeling for Terrestrial Modeling

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

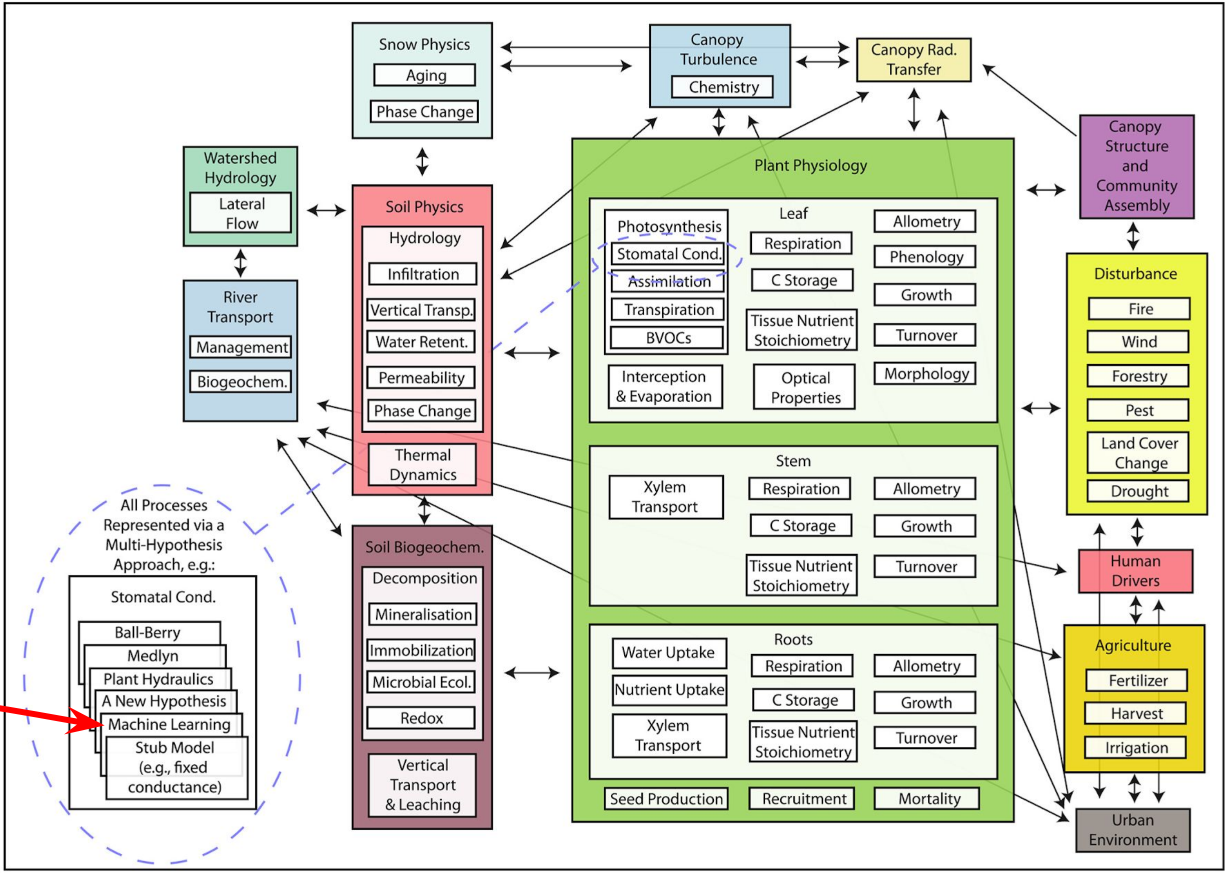
- Multiple hypotheses
- Many leaf-level measurements
- Most computationally intensive part of the land model



(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.



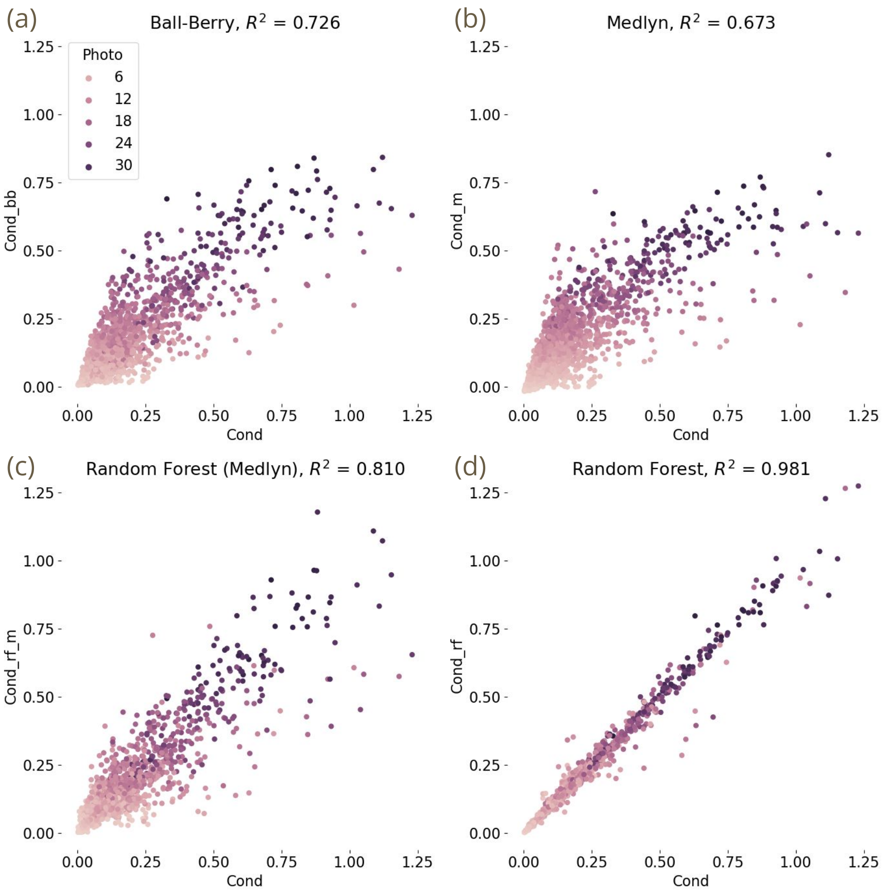
(a) Process Schematic of a Possible Full-Complexity Configuration of a Land Surface Model

(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)

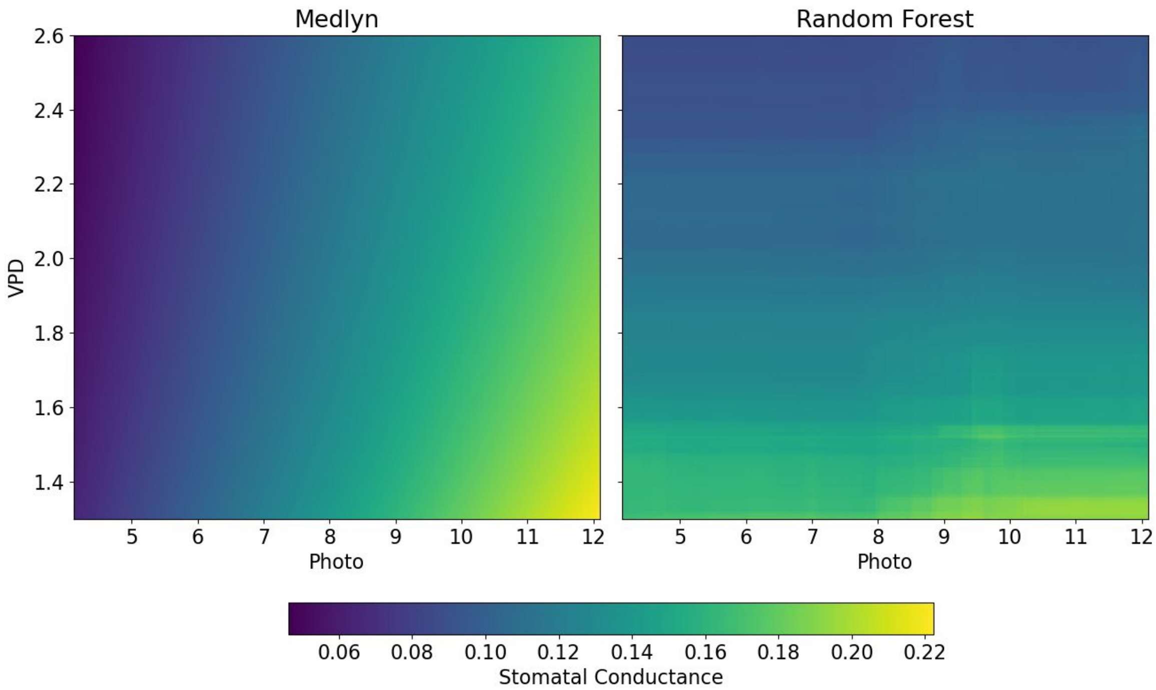


Hybrid Modeling of Photosynthesis and Ecohydrology

- 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

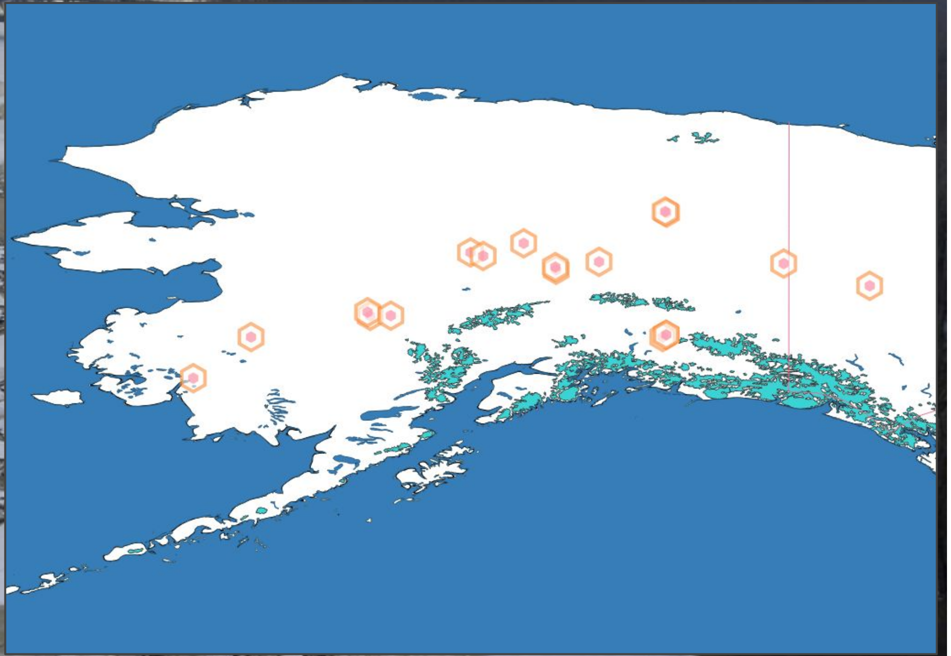
- These discontinuities are likely to have numerical consequences when attempting to couple a ML parameterization into a hybrid empirical / ML Earth system model



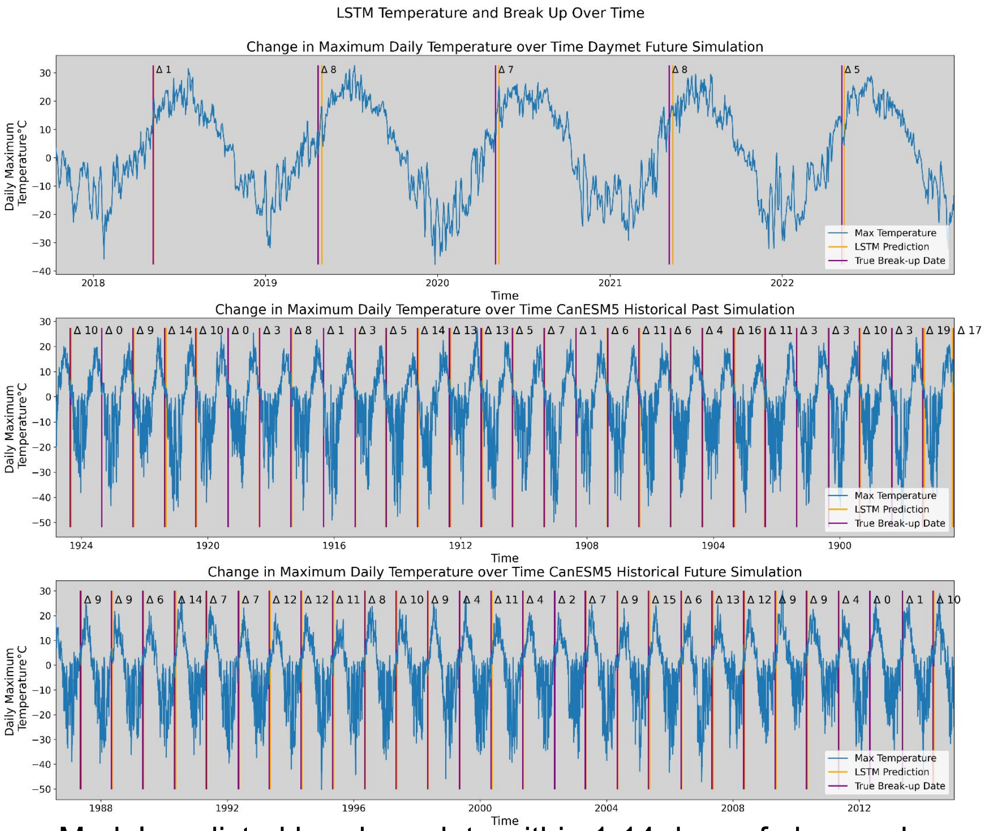
(Massoud, Collier, et al. in prep)

Forecasting River Ice Breakup using LSTM

- Study sites were selected at long term river ice monitoring stations in Yukon river basin.
- We developed Long Short Term Memory (LSTM) 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)

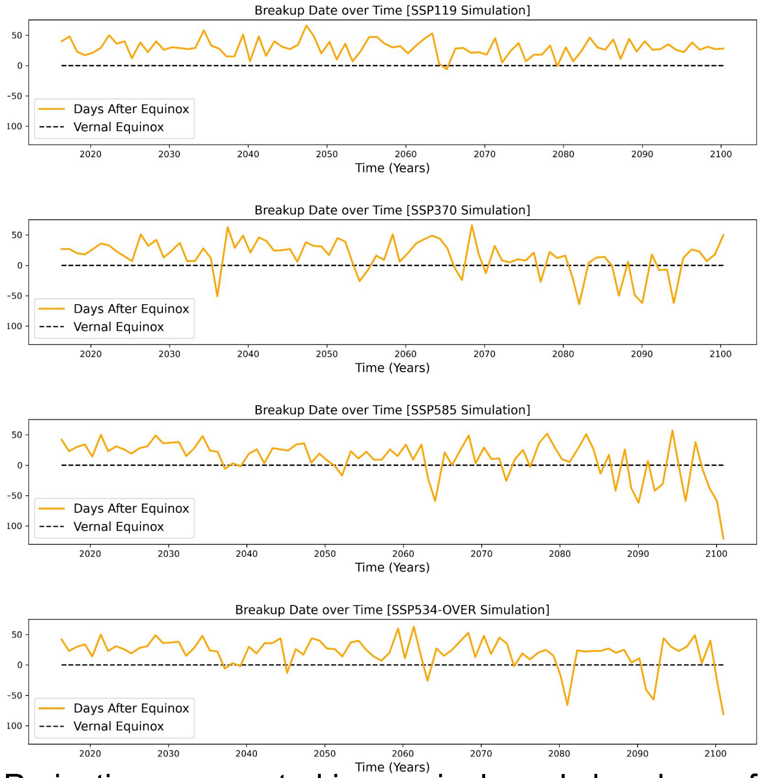


Break-up date predictions for historical period



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.

AI4ESP

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

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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

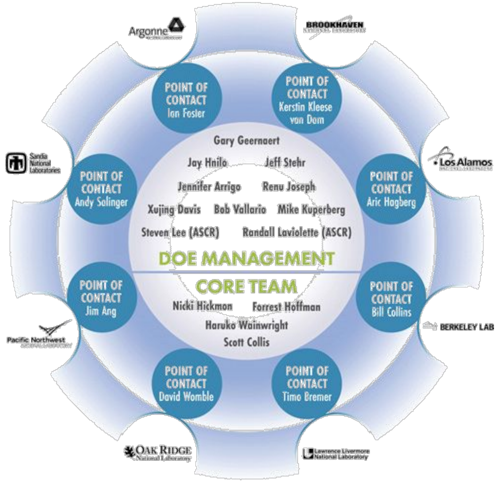
- Data Acquisition
- Neural Networks
- Surrogate models and emulators
- Knowledge-Informed Machine Learning
- Hybrid Modeling
- Explainable/Interpretable/Trustworthy AI
- Knowledge Discovery & Statistical Learning
- AI Architectures and Co-design

Workshop Report

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

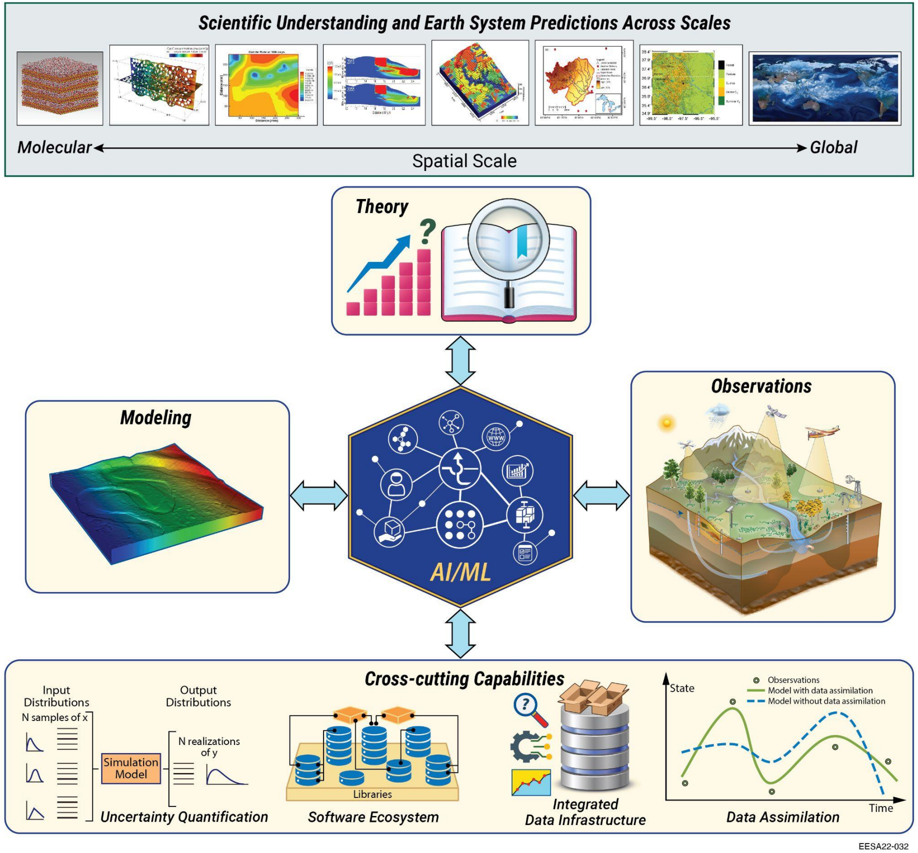
AMS Special Collection

- Open submissions for new AI for the Earth Systems journal



AI4ESP

AI4ESP WORKSHOP HIGHLIGHTS



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

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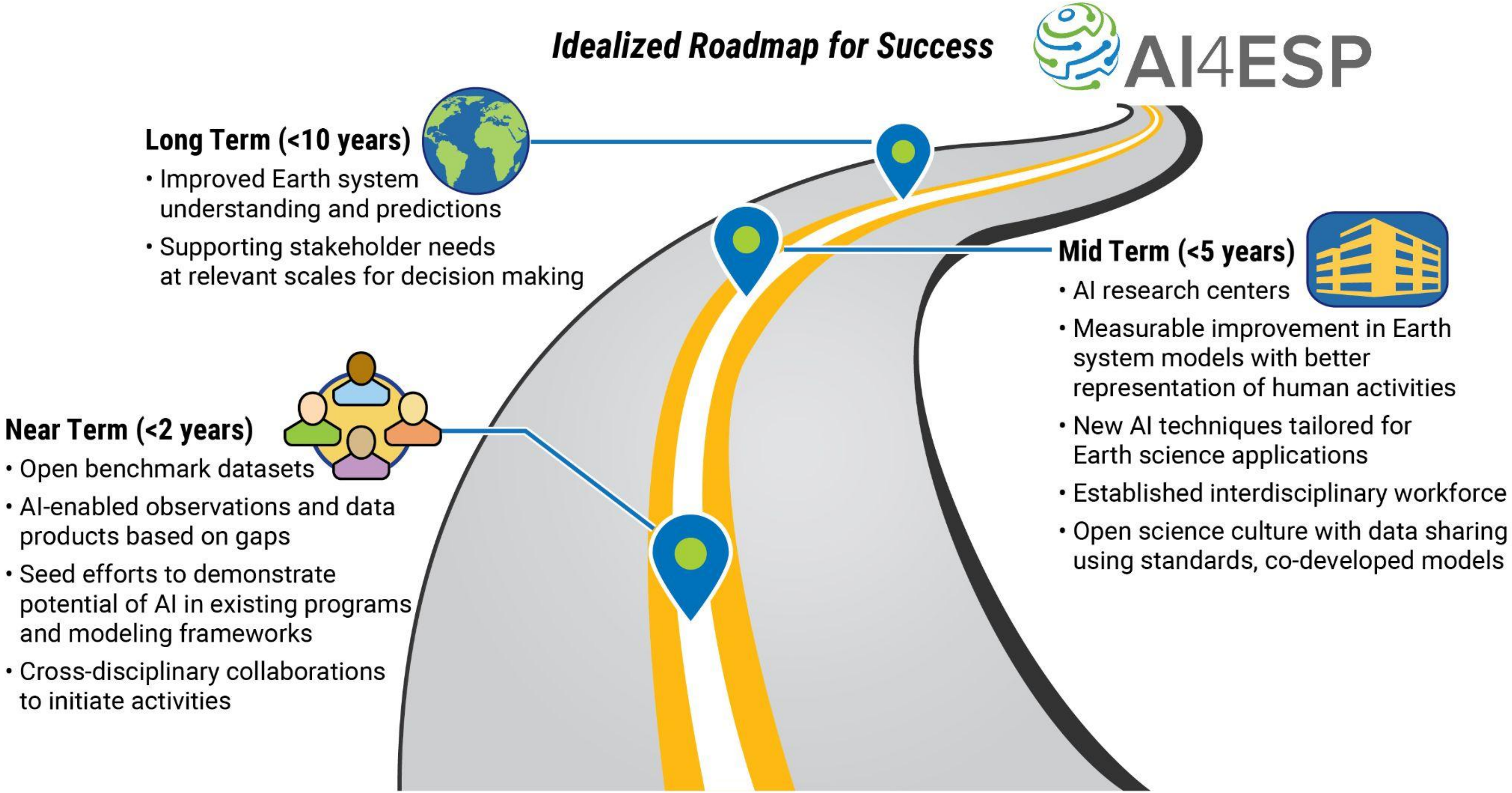
AI4ESP WORKSHOP HIGHLIGHTS



Highlights Across All Sessions

Science

- AI/ML can accelerate next-generation integrated models to support decision-making that incorporate complex natural and human processes at sufficient resolutions
- Broad consensus on need for deep integration of process-based and ML models (hybrid models)
- Challenges: scaling, sub-grid representation, model calibration/UQ, extreme events, human systems
- Data gaps are vast – more observations informed by model needs, AI-ready products
- Results must be robust, explainable, & trustworthy

Data, Software, Infrastructure

- Need benchmark data and model intercomparison approaches
- Computational infrastructure for integration of process & ML models, data assimilation and synthesis
- Use ML to accelerate data-model and model-observation pipelines

Culture

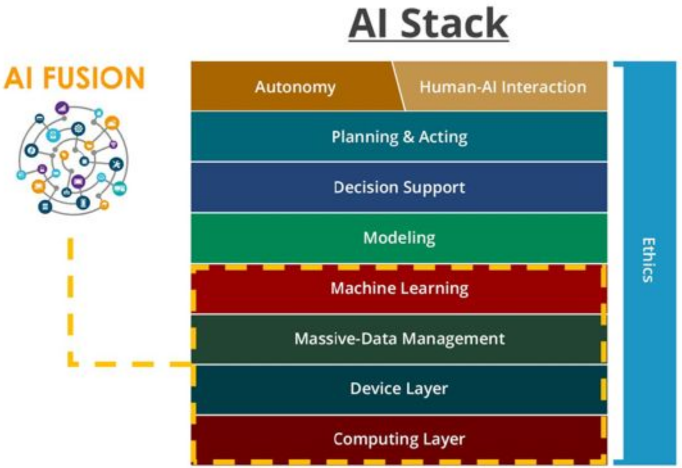
- Workforce development across domain and computational scientists
- Interdisciplinary research centers focused on AI4ESP

AI4ESP WORKSHOP HIGHLIGHTS

Codesign Is Critical

Codesign advanced computing, software, hybrid ML/physical models, observations and future Earth system modeling capabilities

- Common/consistent language & format
- Merged products (standardization, interoperability)
- Adaptive data & parameter selection
- Computation using large datasets without moving
- Specialized AI/ML code & architecture
- Training and benchmarking datasets and hybrid model design



College of Engineering, Carnegie Mellon University

AI4ESP WORKSHOP HIGHLIGHTS

Infrastructure Investment Is Imperative

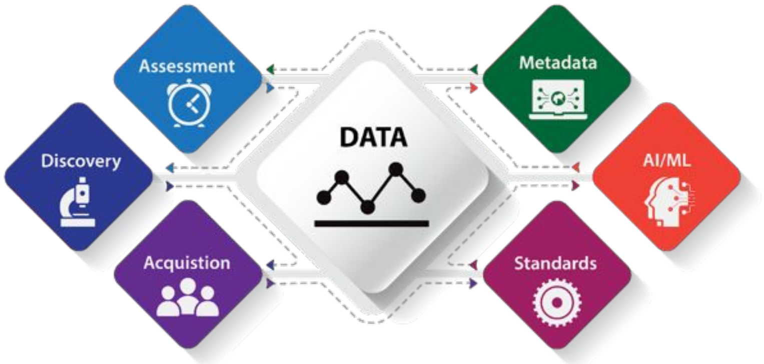
- Workforce development
- Multi-agency/institution coordination, cooperation, collaboration
- Codesign, creation, implementation & maintenance
  - Computational resources
  - Training, benchmarking, & combined datasets
  - AI methodology development
  - Interoperable frameworks for data & hybrid modeling
- FAIR/Equitable data & software practices
- Observations covering normal & capturing rare & extreme events
- Adaptive observatories, data assimilation, & modeling

image from technologynetworks.com

AI4ESP WORKSHOP HIGHLIGHTS

Cultural Change Is Compulsory

- Communities excited to work together
  – need combined purpose and early success
- Existing & upcoming workforce development
- Common terminology across groups & scales in AI4ESP space
- Transfer learning for different domains & scales
- Achieve & maintain FAIR, equitable data access
- Open science community effort pulling in an ultimately singular direction
- Environmental justice throughout the system

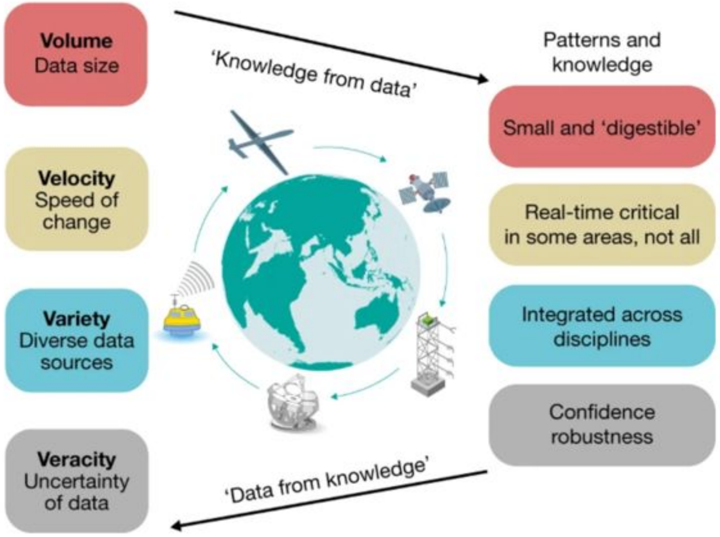


Modular Data Ecosystem to enable data interoperability for AI. Courtesy of Prakash & Serbin

AI4ESP WORKSHOP HIGHLIGHTS

Uncertainty Quantification & Propagation Is Underlying

- Digital twin mindset
- Common understanding of uncertainty
- Defined uncertainty
- Capture beginning with instrument/sensor calibration/operation
- Propagation requires formatting and transfer standards
- Assimilation, parameterization, surrogate, emulator, hybrid modeling

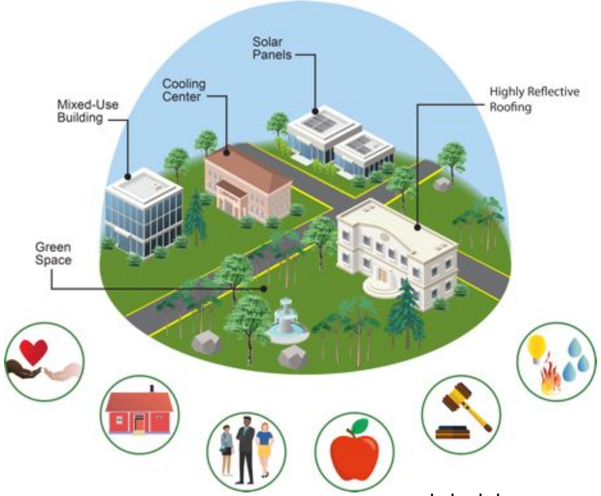


Data challenges in the earth sciences: different data sources, small data / big data challenges, and uncertainty in the data. Figure taken from (Reichstein, M. et al. 2019)

AI4ESP WORKSHOP HIGHLIGHTS

Human System Integration Is Significant

- Inclusion of complex human processes & decisions
- Capture complex feedbacks between all components
- Build decision-relevant process models
- Ethically sensitive data synthesis and gap filling
- Representation of human systems and dynamics in models
- Results must be robust, explainable, & trustworthy
- Results must be shared efficiently (both positive & negative)



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THANK YOU