U.S. DEPARTMENT OF ENERGY
Office of Science

Exploiting Artificial Intelligence for Advancing Earth and Environmental System Science

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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 evaluate and benchmark model results
- Explosive data growth and the promise of discovery through data-driven modeling necessitate new methods for feature extraction, change detection, data assimilation, simulation, and analysis

Summit at Oak Ridge National Laboratory, #2 fastest supercomputer on the [TOP500](TOP500) List (June 2021).

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

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

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

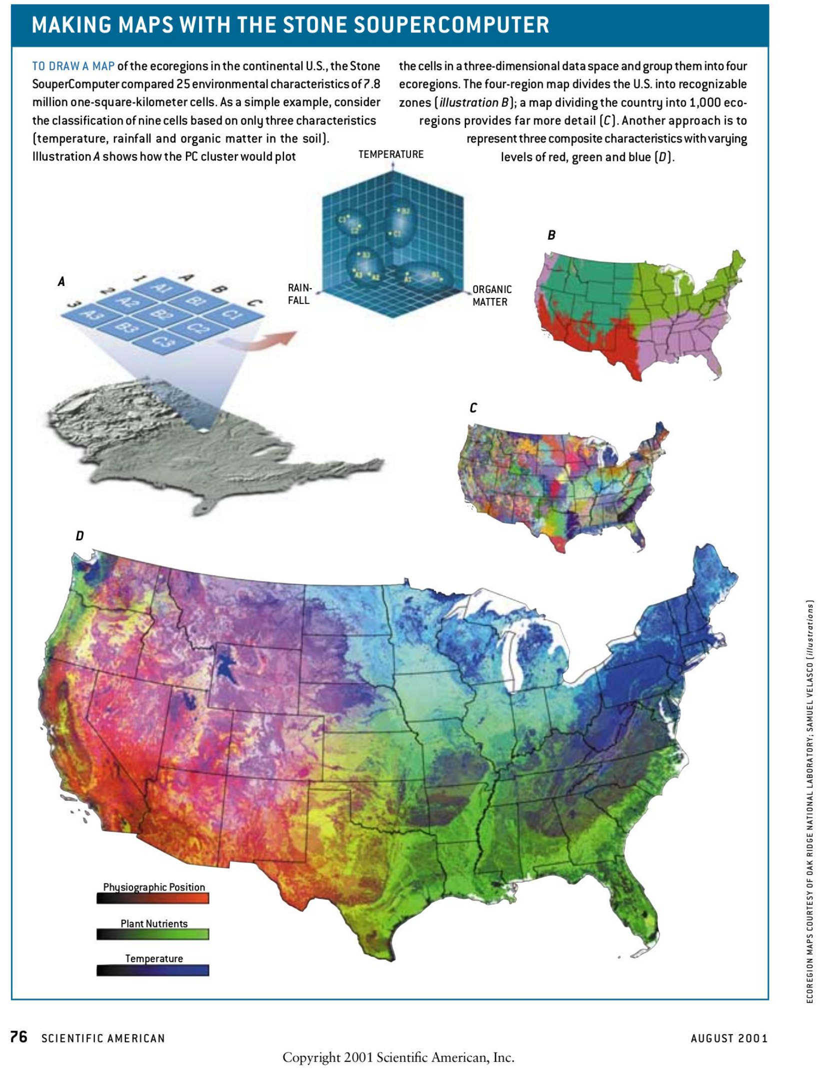
Photographs by Kay Chernush

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

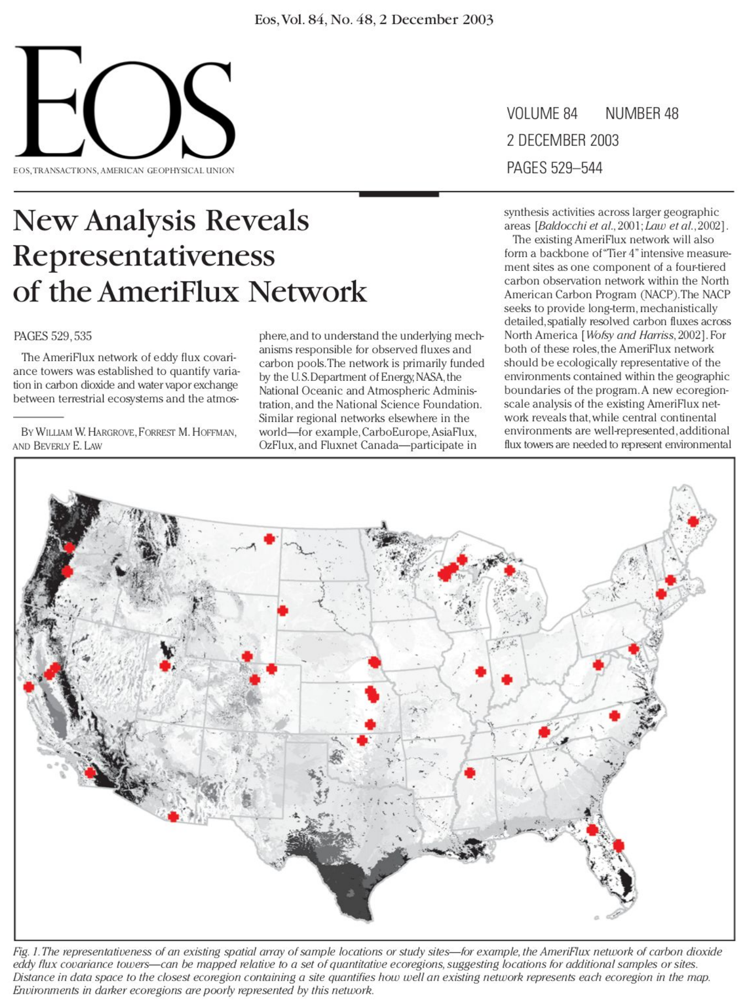


MAKING MAPS WITH THE STONE SOUPERCOMPUTER

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 ecoregions 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/


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

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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.

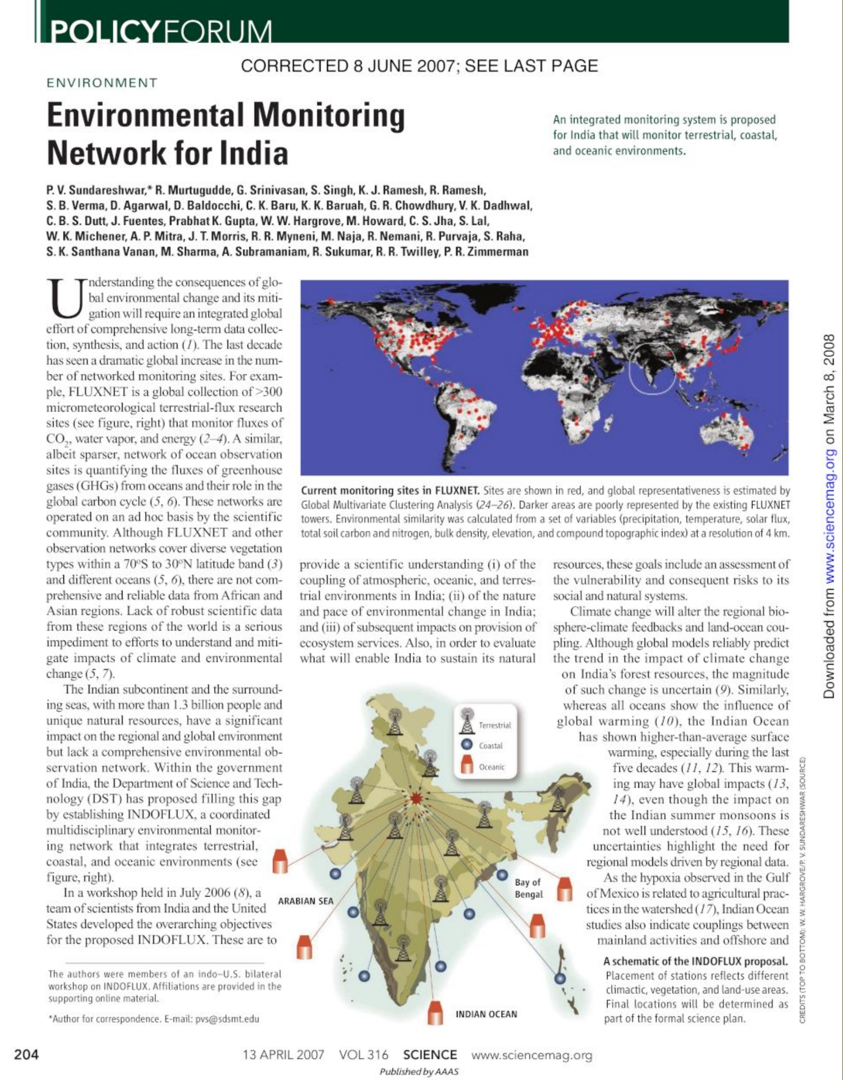
Network Representativeness

- 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

- **Professor Vinay Kumar Dadhwal** showed this paper in his Keynote Lecture yesterday
- 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


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.

Terrestrial
Coastal
Oceanic
ARABIAN SEA
Bay of Bengal
INDIAN OCEAN

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.

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

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

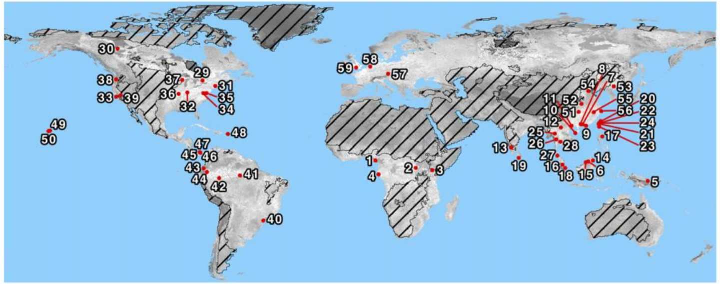

Fig. 1 Map of the CTFS-ForestGEO network illustrating its representation of bioclimatic, edaphic, and topographic conditions globally. Site numbers correspond to ID# in Table 2. Shading indicates how well the network of sites represents the suite of environmental factors included in the analysis; light-colored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

Representativeness for Alaska

Data Layers

Table: 37 characteristics averaged for the present (2000–2009) and the future (2090–2099).

Description	Number/Name	Units	Source
Monthly mean air temperature	12	°C	GCM
Monthly mean precipitation	12	mm	GCM
Day of freeze	mean	day of year	GCM
	standard deviation	days	
Day of thaw	mean	day of year	GCM
	standard deviation	days	
Length of growing season	mean	days	GCM
	standard deviation	days	
Maximum active layer thickness	1	m	GIPL
Warming effect of snow	1	°C	GIPL
Mean annual ground temperature at bottom of active layer	1	°C	GIPL
Mean annual ground surface temperature	1	°C	GIPL
Thermal offset	1	°C	GIPL
Limnicity	1	%	NHD
Elevation	1	m	SRTM

Hoffman, F. M., J. Kumar, R. T. Mills, and W. W. Hargrove (2013), Representativeness-Based Sampling Network Design for the State of Alaska, *Landscape Ecol.*, 28(8):1567–1586, doi:10.1007/s10980-013-9902-0.

Landscape Ecol (2013) 28:1567–1586
DOI 10.1007/s10980-013-9902-0

RESEARCH ARTICLE

Representativeness-based sampling network design for the State of Alaska

Forrest M. Hoffman · Jitendra Kumar · Richard T. Mills · William W. Hargrove

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Abstract Resource and logistical constraints limit the frequency and extent of environmental observations, particularly in the Arctic, necessitating the development of a systematic sampling strategy to maximize coverage and objectively represent environmental variability at desired scales. A quantitative methodology for stratifying sampling domains, informing site selection, and determining the representativeness of measurement sites and networks is described here. Multivariate spatiotemporal clustering was applied to down-scaled general circulation model results and data for the State of Alaska at 4 km^2 resolution to define multiple sets of ecoregions across two decadal time periods. Maps of ecoregions for the present (2000–2009) and future (2090–2099) were produced, showing how combinations of 37 characteristics are distributed and how they may shift in the future. Representative sampling locations are identified on present and future ecoregion maps. A representativeness metric was developed, and representativeness maps for eight candidate sampling locations were produced. This metric was used to characterize the environmental similarity of each site. This analysis provides model-inspired insights into optimal sampling strategies, offers a framework for up-scaling measurements, and provides a down-scaling approach for integration of models and measurements. These techniques can be applied at different spatial and temporal scales to meet the needs of individual measurement campaigns.

Keywords Ecoregions · Representativeness · Network design · Cluster analysis · Alaska · Permafrost

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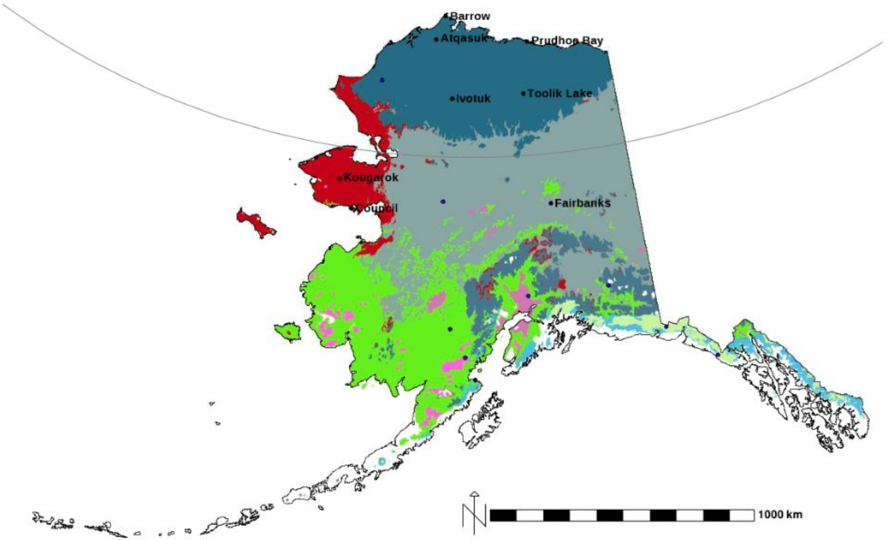
Introduction

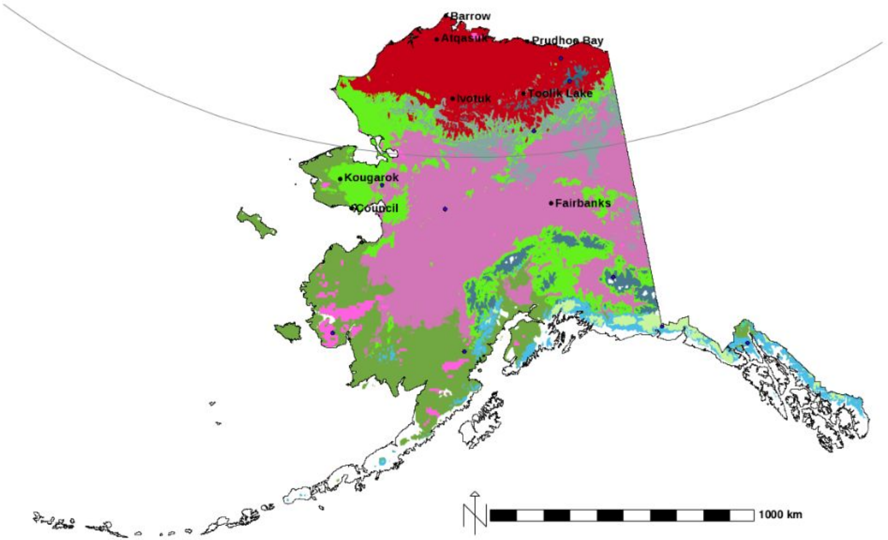
The Arctic contains vast amounts of frozen water in the form of sea ice, snow, glaciers, and permafrost. Extended areas of permafrost in the Arctic contain soil organic carbon that is equivalent to twice the size of the atmospheric carbon pool, and this large stabilized

10 Alaska Ecoregions, Present and Future

(Hoffman et al., 2013)



2000–2009

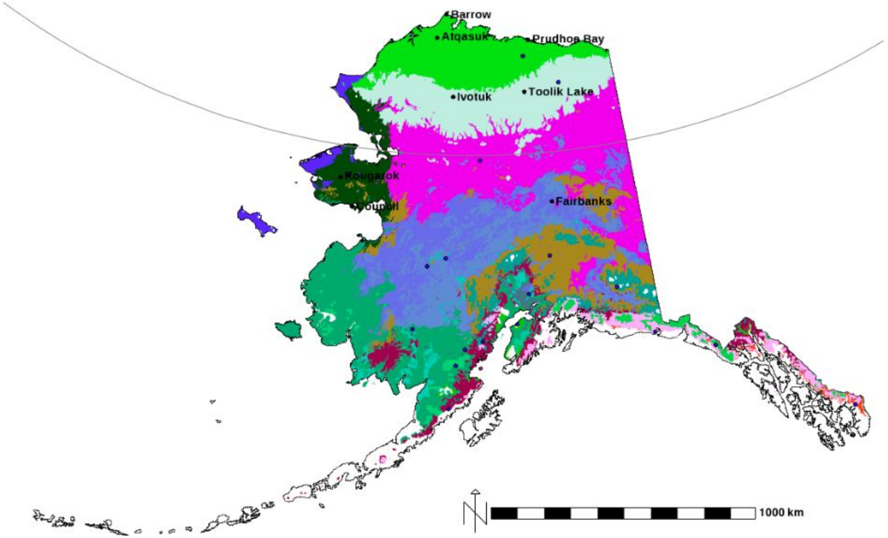


2090–2099

- Since the random colors are the same in both maps, a change in color represents an environmental change between the present and the future.
- At this level of division, the conditions in the large boreal forest become compressed onto the Brooks Range and the conditions on the Seward Peninsula “migrate” to the North Slope.

20 Alaska Ecoregions, Present and Future

(Hoffman et al., 2013)



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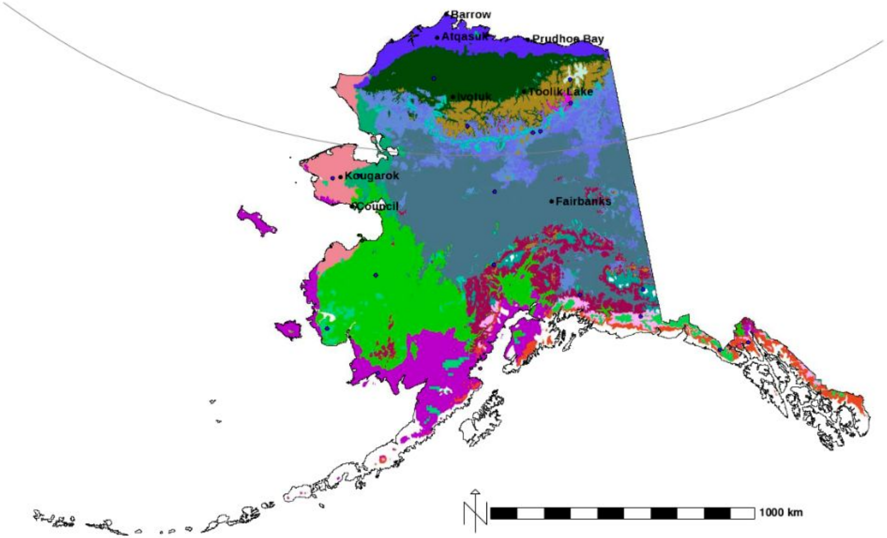


2090–2099

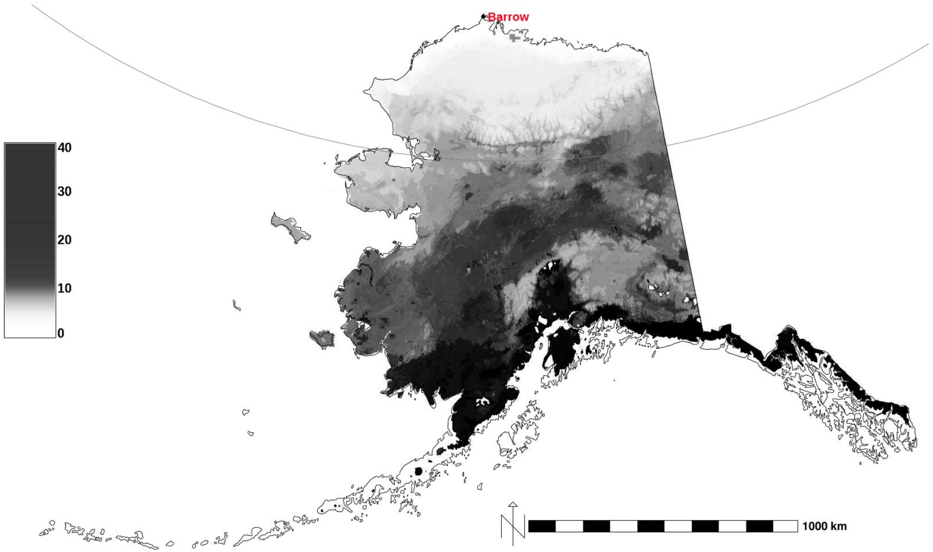
- Since the random colors are the same in both maps, a change in color represents an environmental change between the present and the future.
- At this level of division, the two primary regions of the Seward Peninsula and that of the northern boreal forest replace the two regions on the North Slope almost entirely.

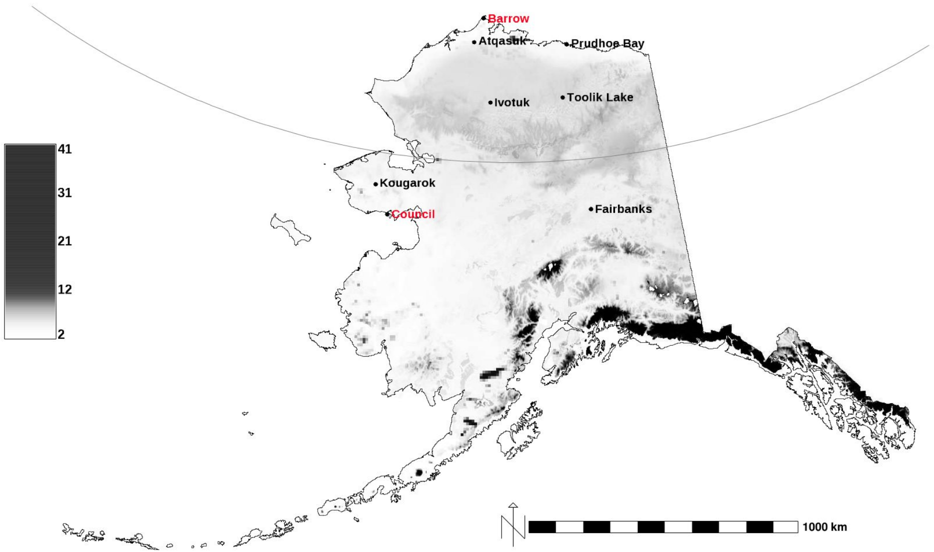
Sampling Site Representativeness

- This representativeness analysis uses the standardized *n*-dimensional data space formed from all input data layers
- In this data space, the Euclidean distance between a sampling location (like Barrow) and every other point is calculated
- These data space distances are then used to generate grayscale maps showing the similarity, or lack thereof, of every location to the sampling location
- In the subsequent maps, white areas are well represented by the sampling location or network, while dark and black areas as poorly represented by the sampling location or network
- This analysis assumes that the climate surrogates maintain their predictive power and that no significant biological adaptation occurs in the future

Network Representativeness: Barrow vs. Barrow + Council

(Hoffman et al., 2013)





Light-colored regions are well represented and dark-colored regions are poorly represented by the sampling location listed in **red**.

State Space Dissimilarities: 8 Sites, Present (2000–2009)

Table: Site state space dissimilarities for the present (2000–2009).

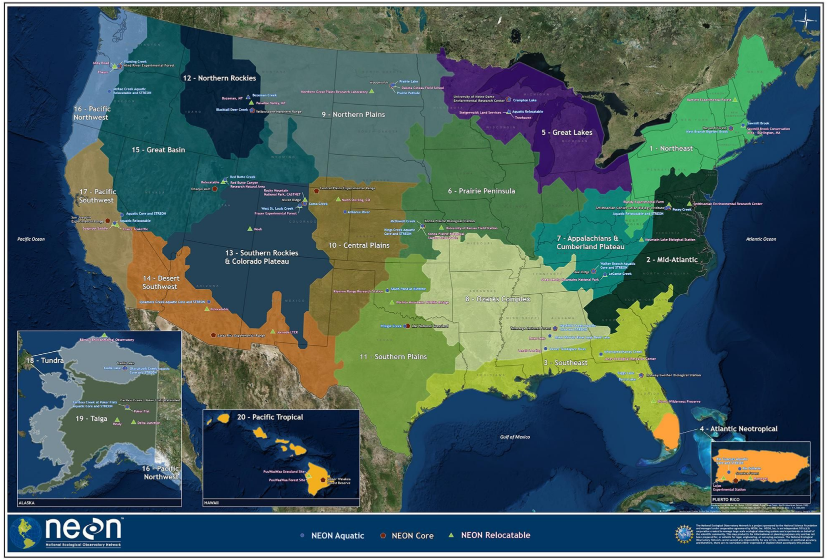
Sites	Council	Atqasuk	Ivotuk	Toolik Lake	Kougarok	Prudhoe Bay	Fairbanks
Barrow	9.13	4.53	5.90	5.87	7.98	3.57	12.16
Council		8.69	6.37	7.00	2.28	8.15	5.05
Atqasuk			5.18	5.23	7.79	1.74	10.66
Ivotuk				1.81	5.83	4.48	7.90
Toolik Lake					6.47	4.65	8.70
Kougarok						7.25	5.57
Prudhoe Bay							10.38

State Space Dissimilarities: 8 Sites, Present and Future

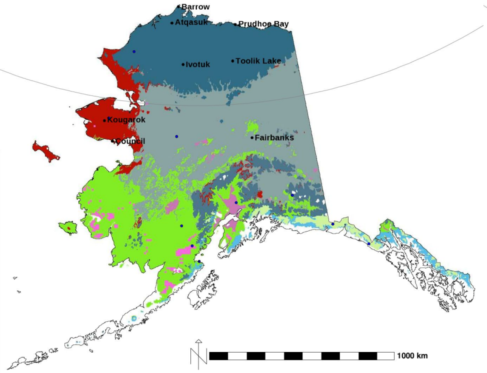
Table: Site state space dissimilarities between the present (2000–2009) and the future (2090–2099).

		Future (2090–2099)							
	Sites	Barrow	Council	Atqasuk	Ivotuk	Toolik Lake	Kougarok	Prudhoe Bay	Fairbanks
Present (2000–2009)	Barrow	3.31	9.67	4.63	6.05	5.75	9.02	3.69	11.67
	Council	8.38	1.65	8.10	5.91	6.87	3.10	7.45	5.38
	Atqasuk	6.01	9.33	2.42	5.46	5.26	8.97	2.63	10.13
	Ivotuk	7.06	7.17	5.83	1.53	2.05	7.25	4.87	7.40
	Toolik Lake	7.19	7.67	6.07	2.48	1.25	7.70	5.23	8.16
	Kougarok	7.29	3.05	6.92	5.57	6.31	2.51	6.54	5.75
	Prudhoe Bay	5.29	8.80	3.07	4.75	4.69	8.48	1.94	9.81
	Fairbanks	12.02	5.49	10.36	7.83	8.74	6.24	10.10	1.96

Sampling Network Design



NSF’s NEON Sampling Domains



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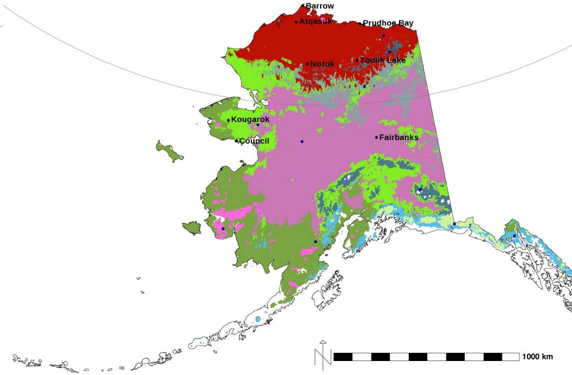
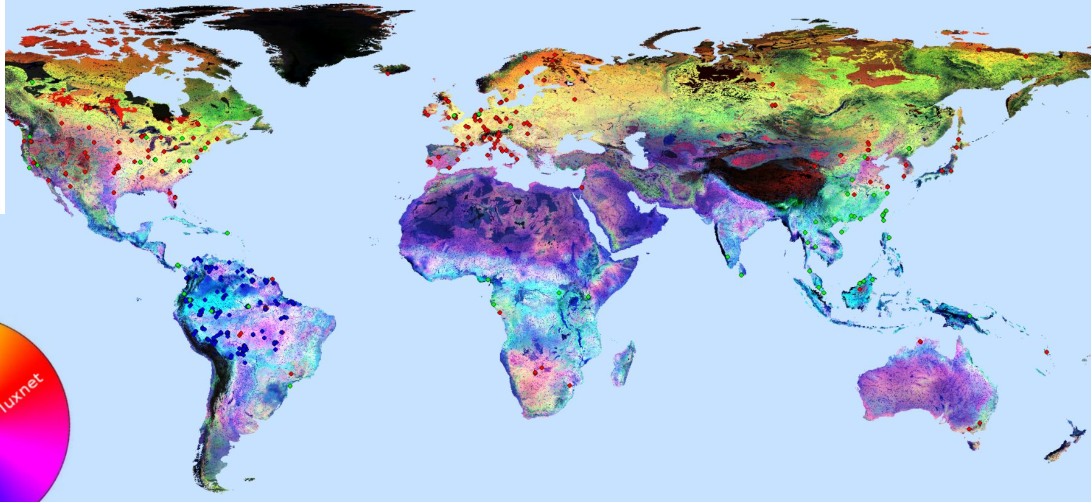
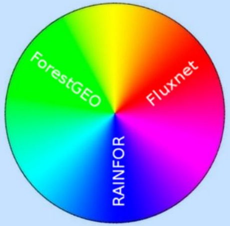


2090–2000

(Hoffman et al., 2013)

Triple-Network Global Representativeness



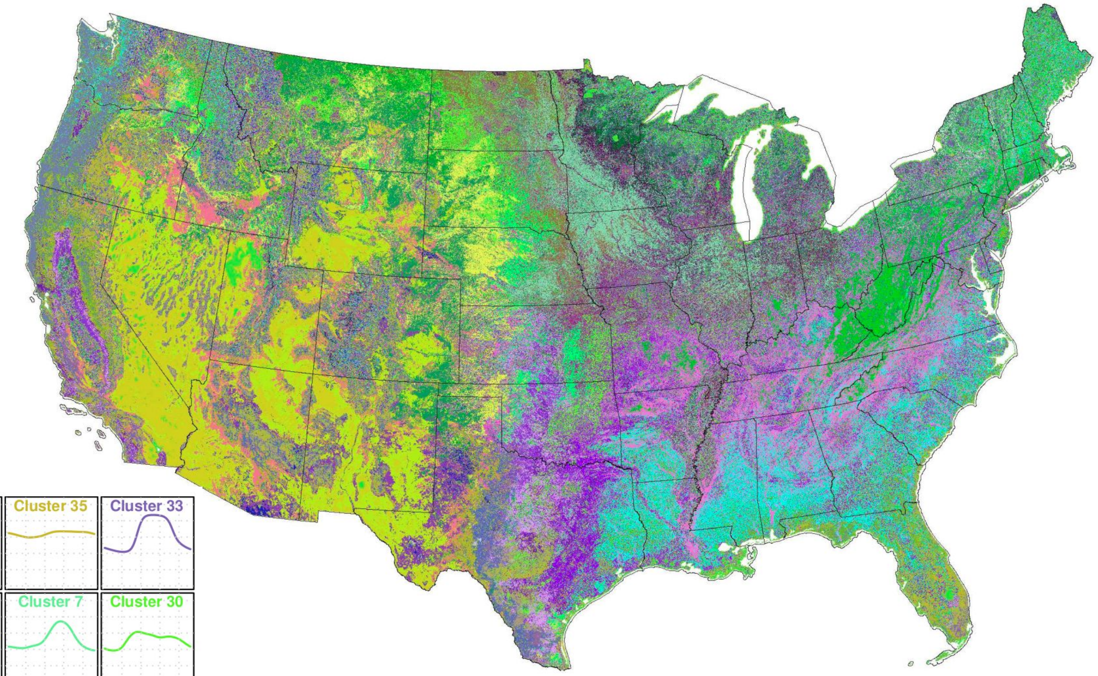


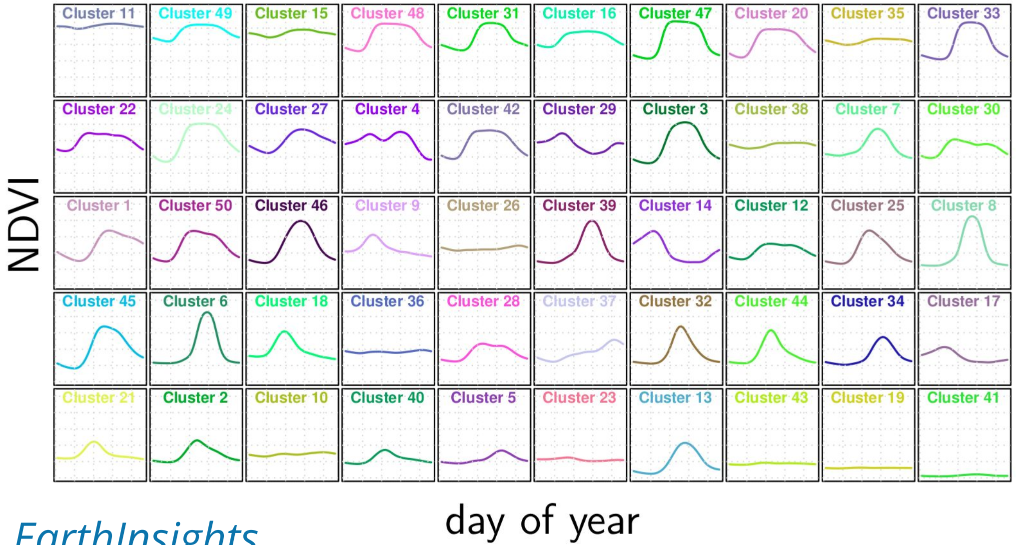
(Maddalena et al., in prep.)

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

50 Phenoregions for year 2012 (Random Colors)

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

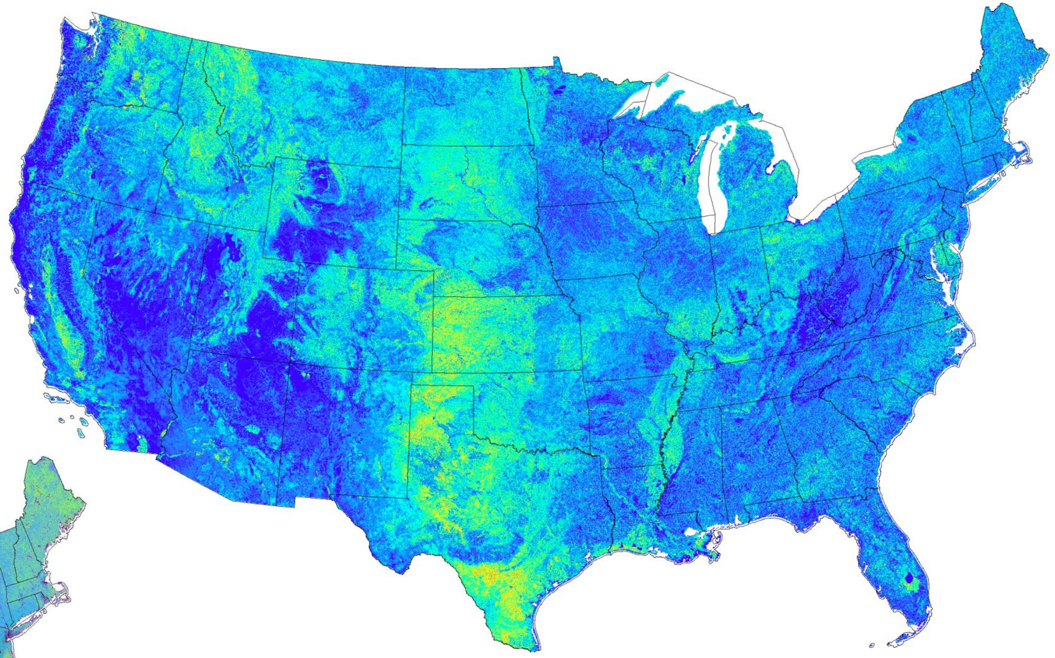


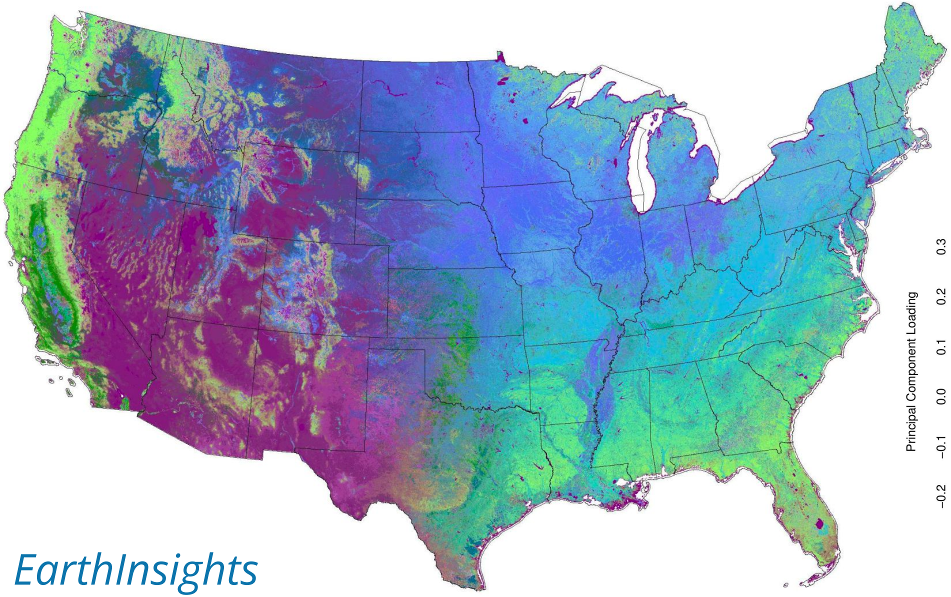


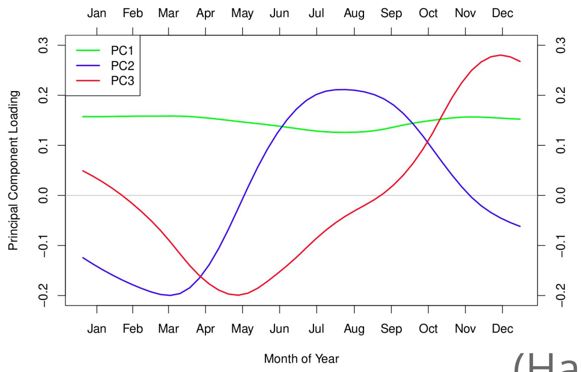
50 Phenoregion Prototypes (Random Colors)

(Hargrove et al., in prep.)

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







Principal Components Analysis

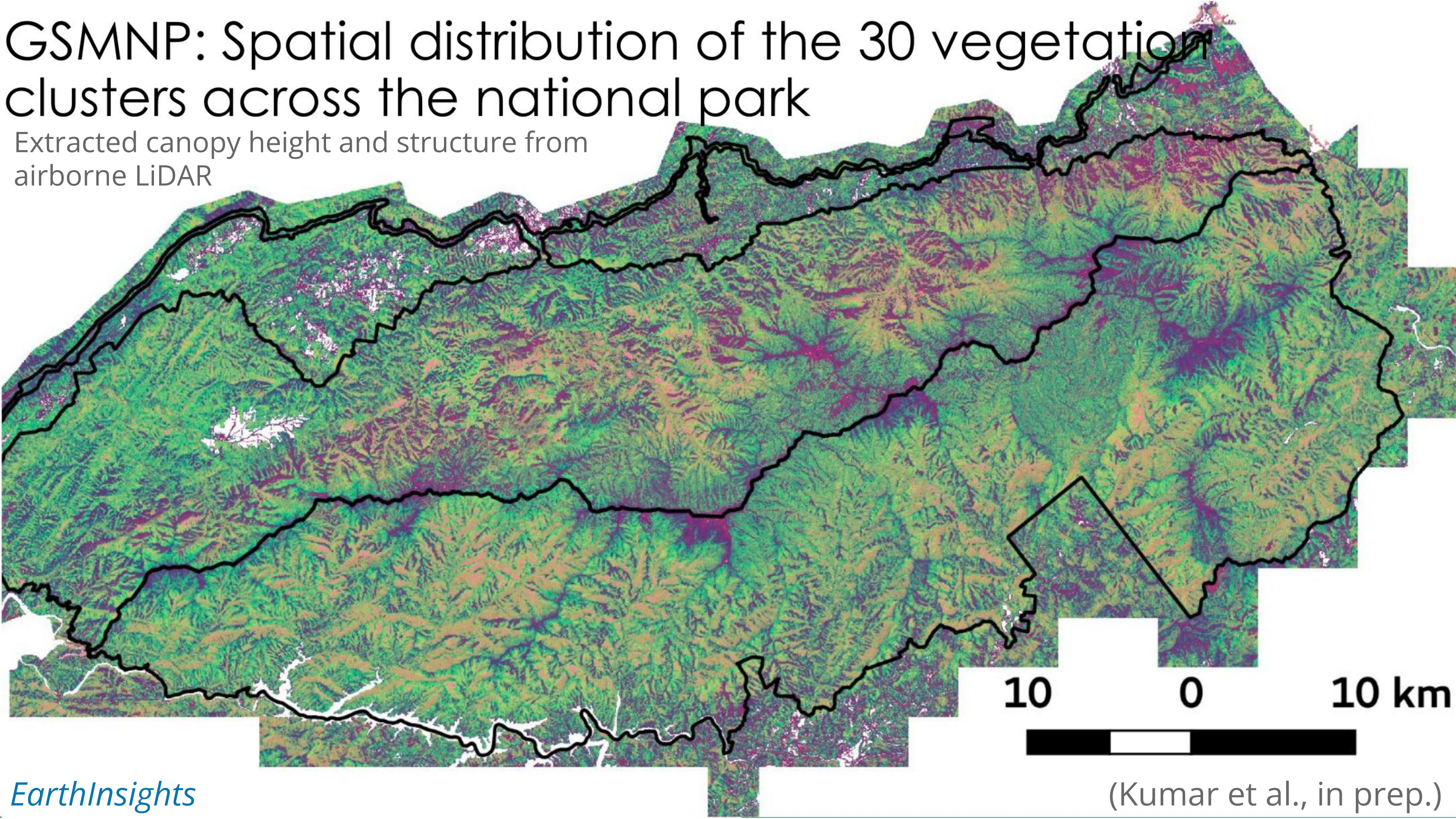
PC1 ~ Evergreen
PC2 ~ Deciduous
PC3 ~ Dry Deciduous

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

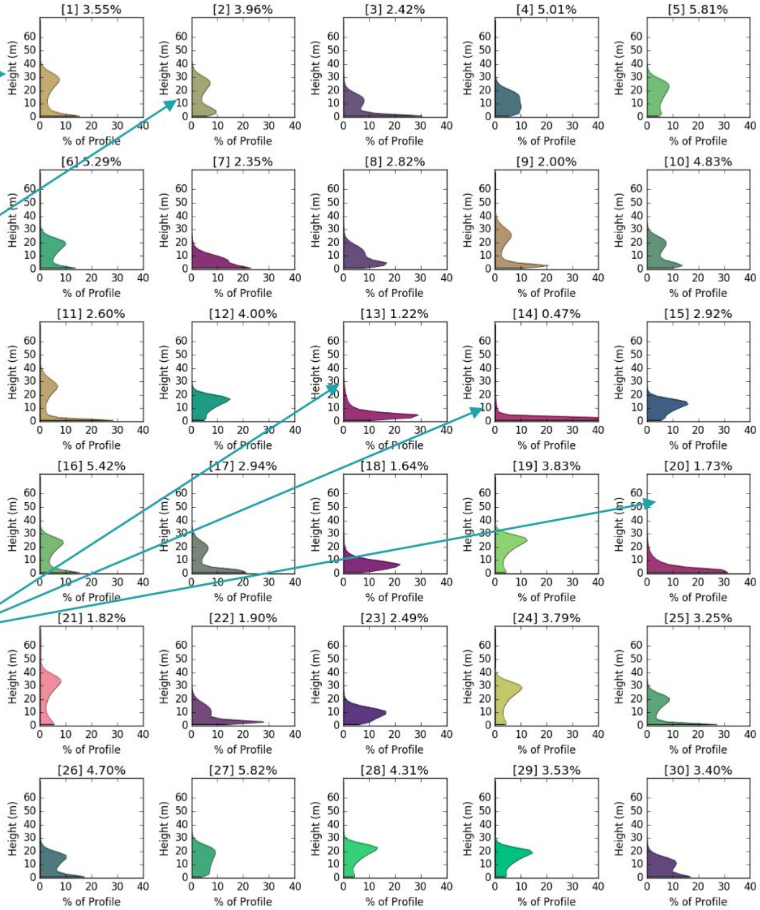
(Kumar et al., in prep.)

GSMNP: 30 representative vertical structures (cluster centroids) identified

tall forests with low understory vegetation

forests with slightly lower mean height with dense understory vegetation

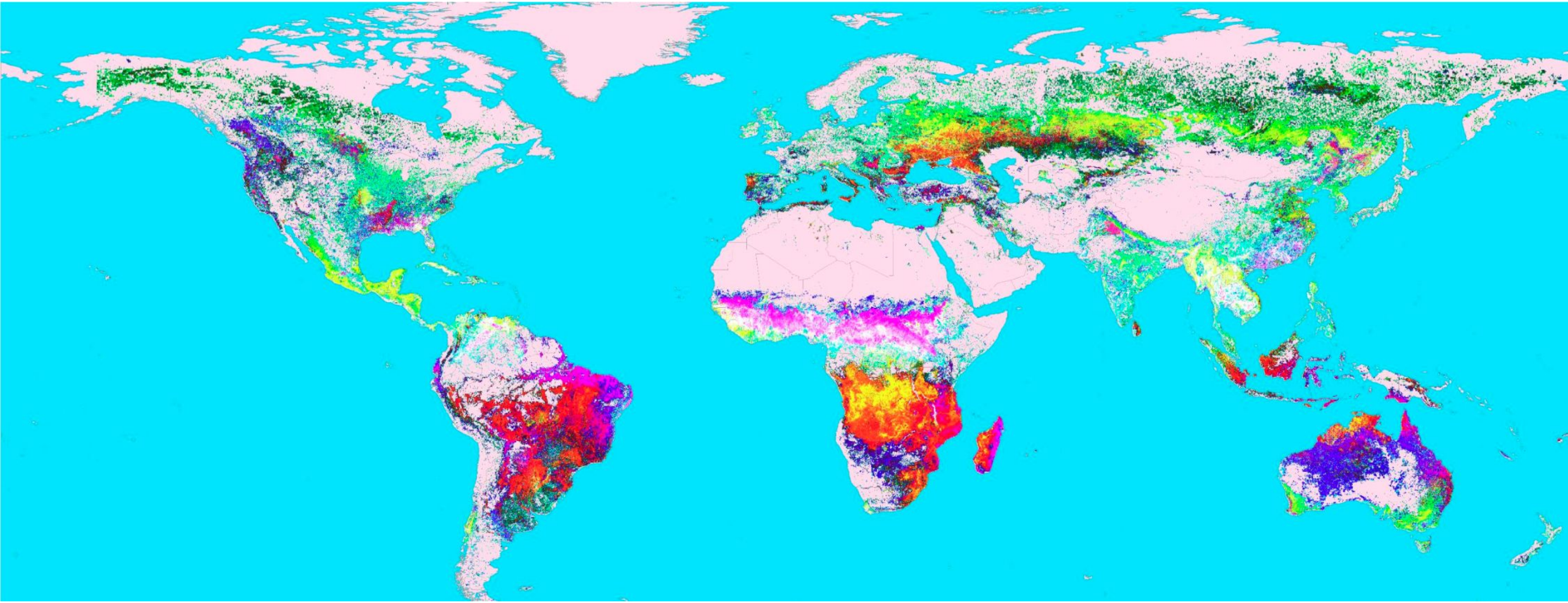
low height grasslands and heath balds that are small in area but distinct landscape type



EarthInsights

(Kumar et al., in prep.)

Global Fire Regimes

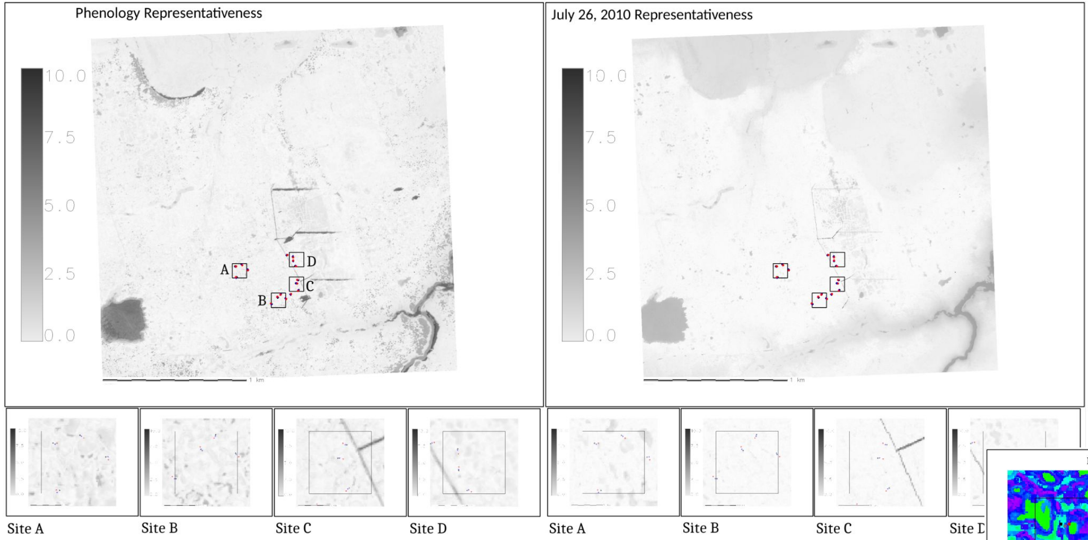


Regions that exhibit similar fire seasonality globally

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

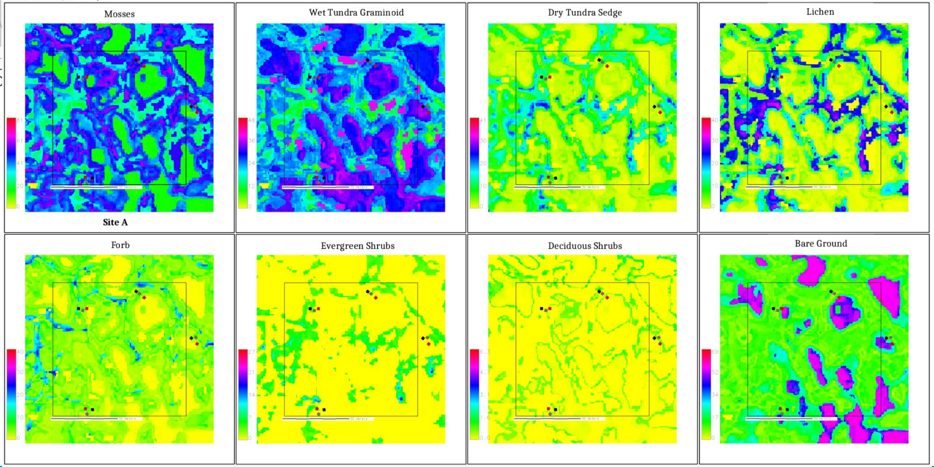
(Norman et al., in prep.)

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

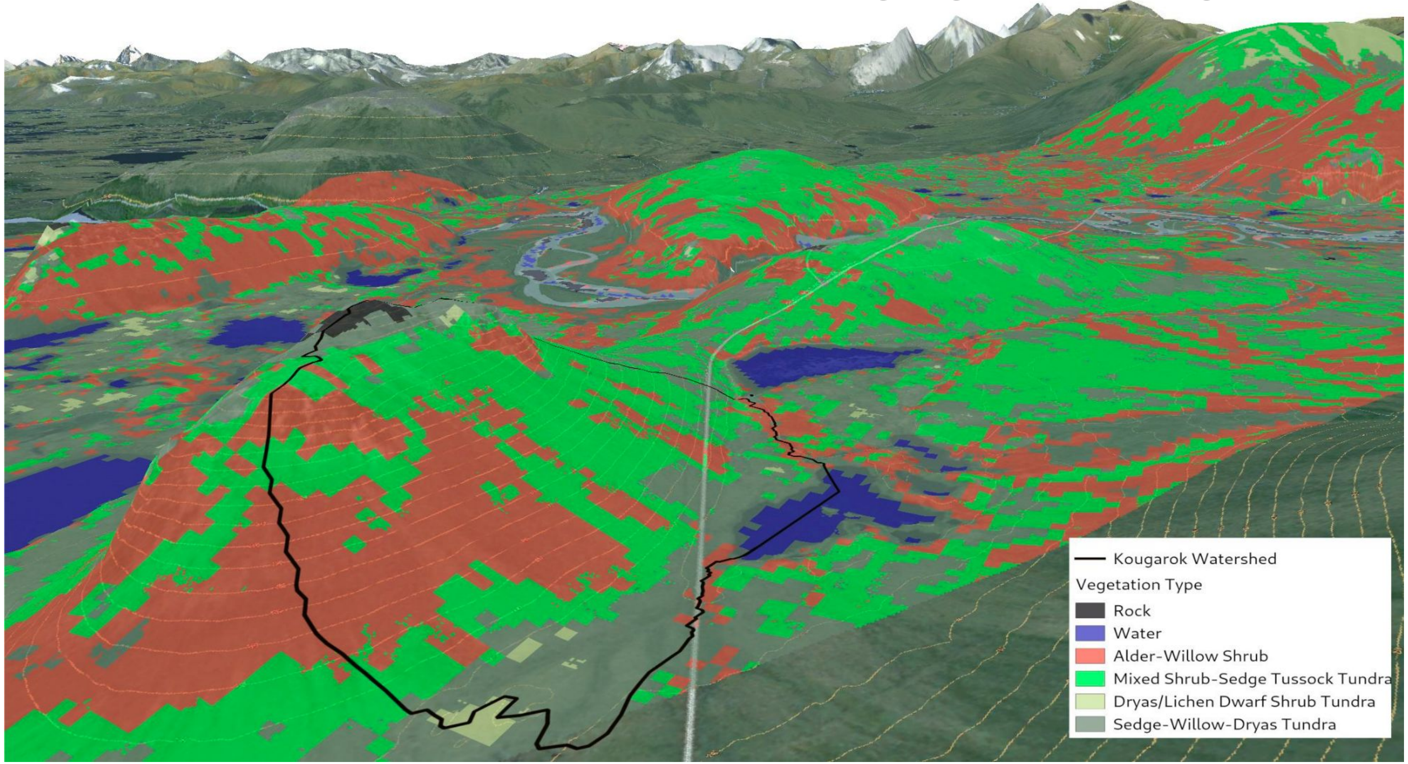


In situ data from field measurement activities inform the development of wide-scale maps of vegetation distribution through inference using remote sensing data as surrogate variables, and relationships with environmental controls can be extracted

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

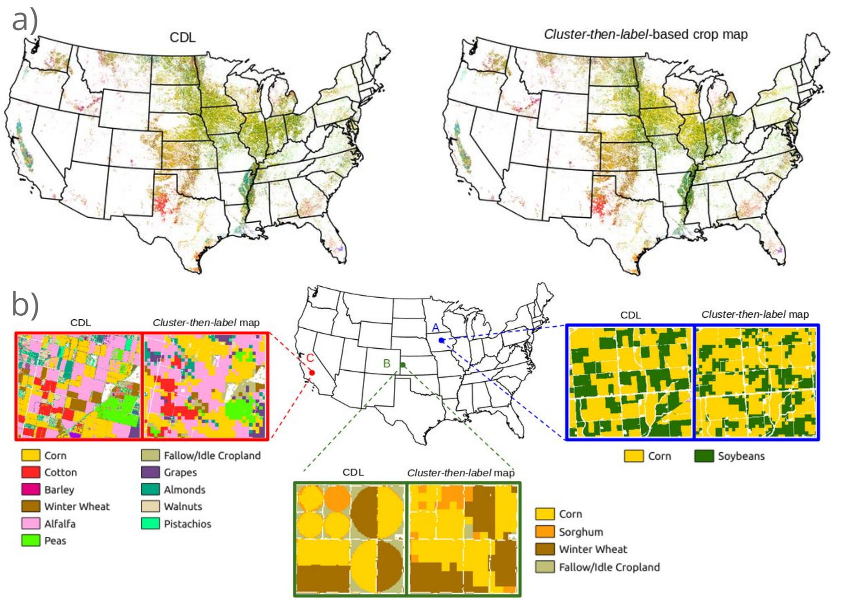
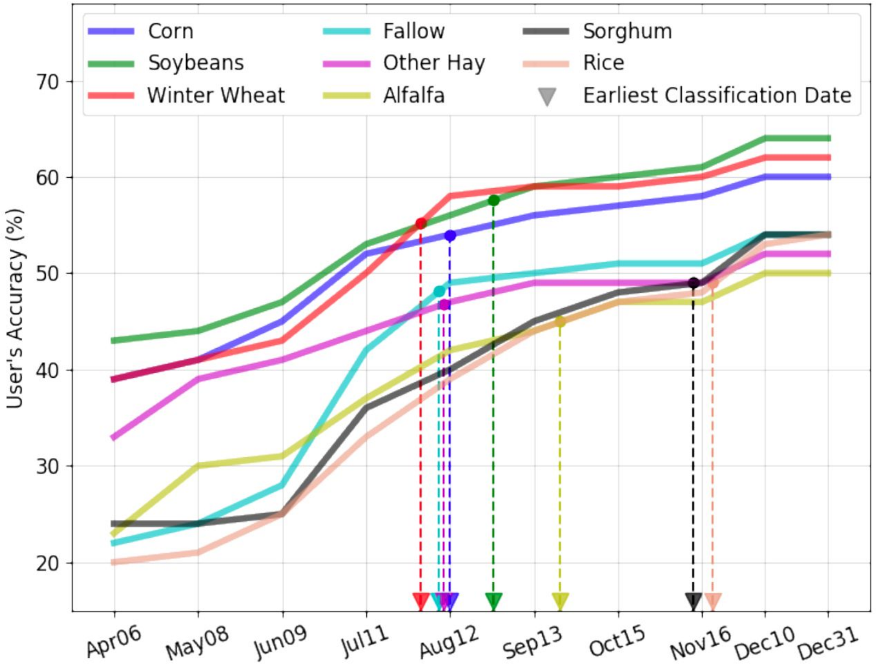


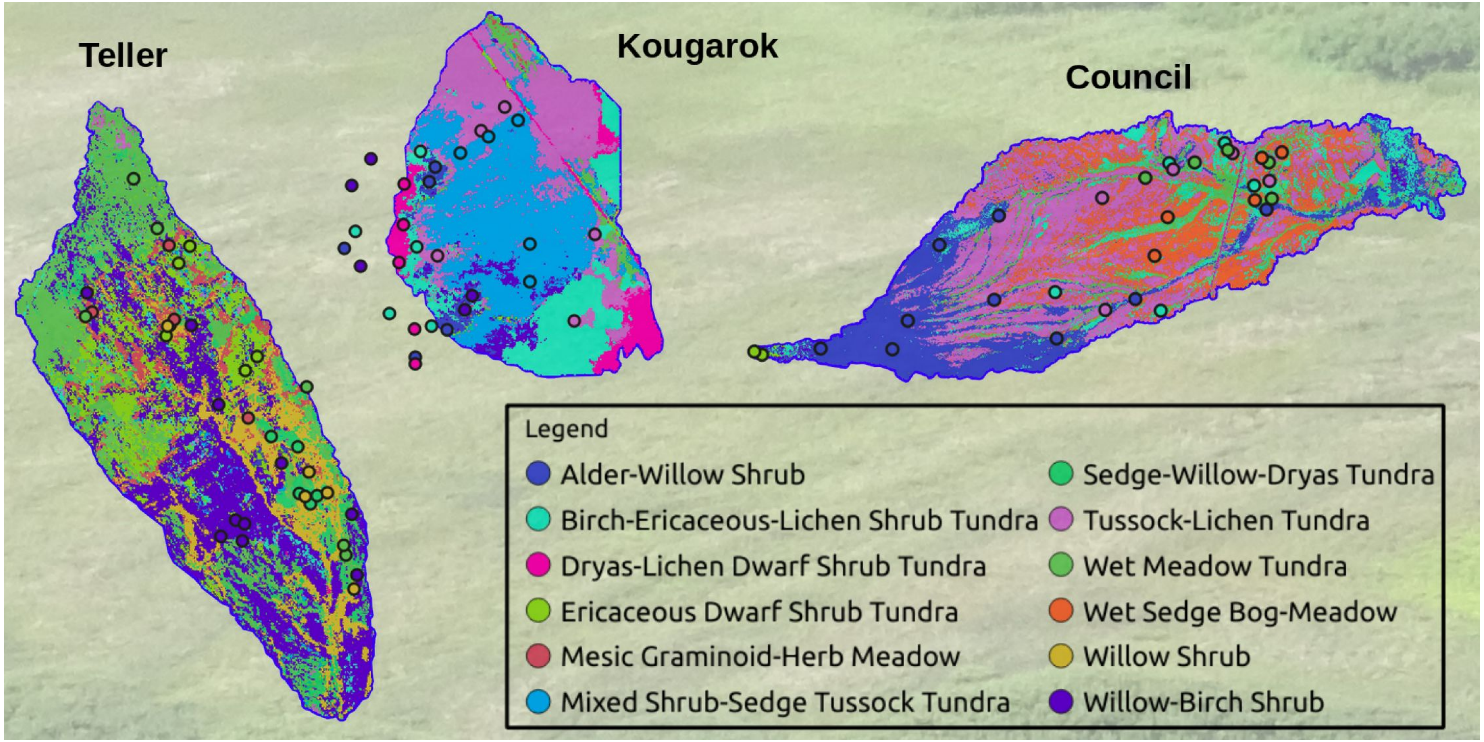
Figure: a) Comparison of cluster-then-label crop map with USDA Crop Data Layer (CDL) shows similar patterns at continental scale. b) Good spatial agreement is found at three selected regions, but cluster-then-label crop maps lack sharpness at field boundaries due to coarser resolution of MODIS data.

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](https://doi.org/10.1016/j.rse.2020.112048).

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



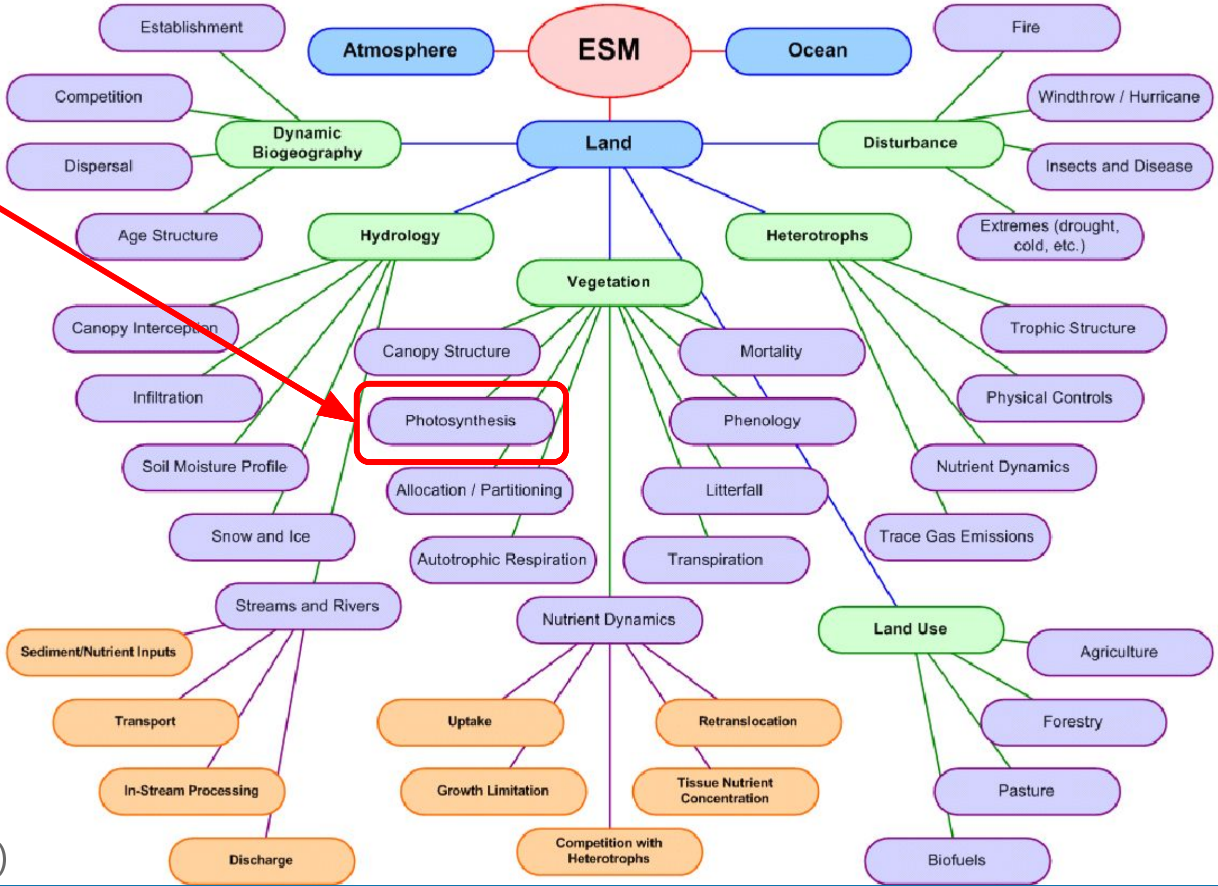
At the watershed scale, vegetation community distribution follows topographic and water controls.
At a fine scale, nutrients limit the distribution of vegetation types.

(Konduri et al., in prep.)

Hybrid ML/Process-based Modeling for Terrestrial Modeling

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

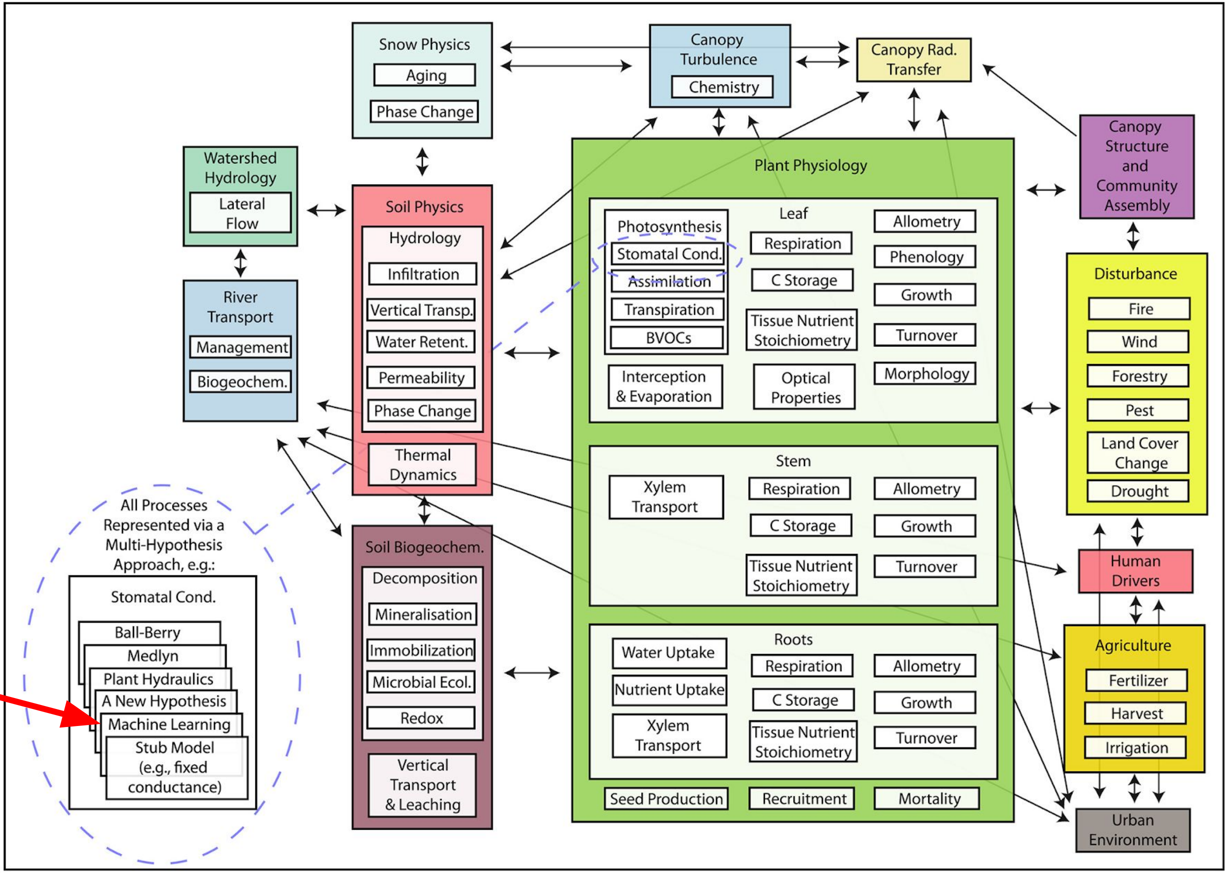
- Multiple hypotheses
- Many leaf-level measurements
- Most computationally intensive part of the land model



(Figure from P. E. Thornton)

Hybrid ML/Process-based Modeling for Terrestrial Modeling

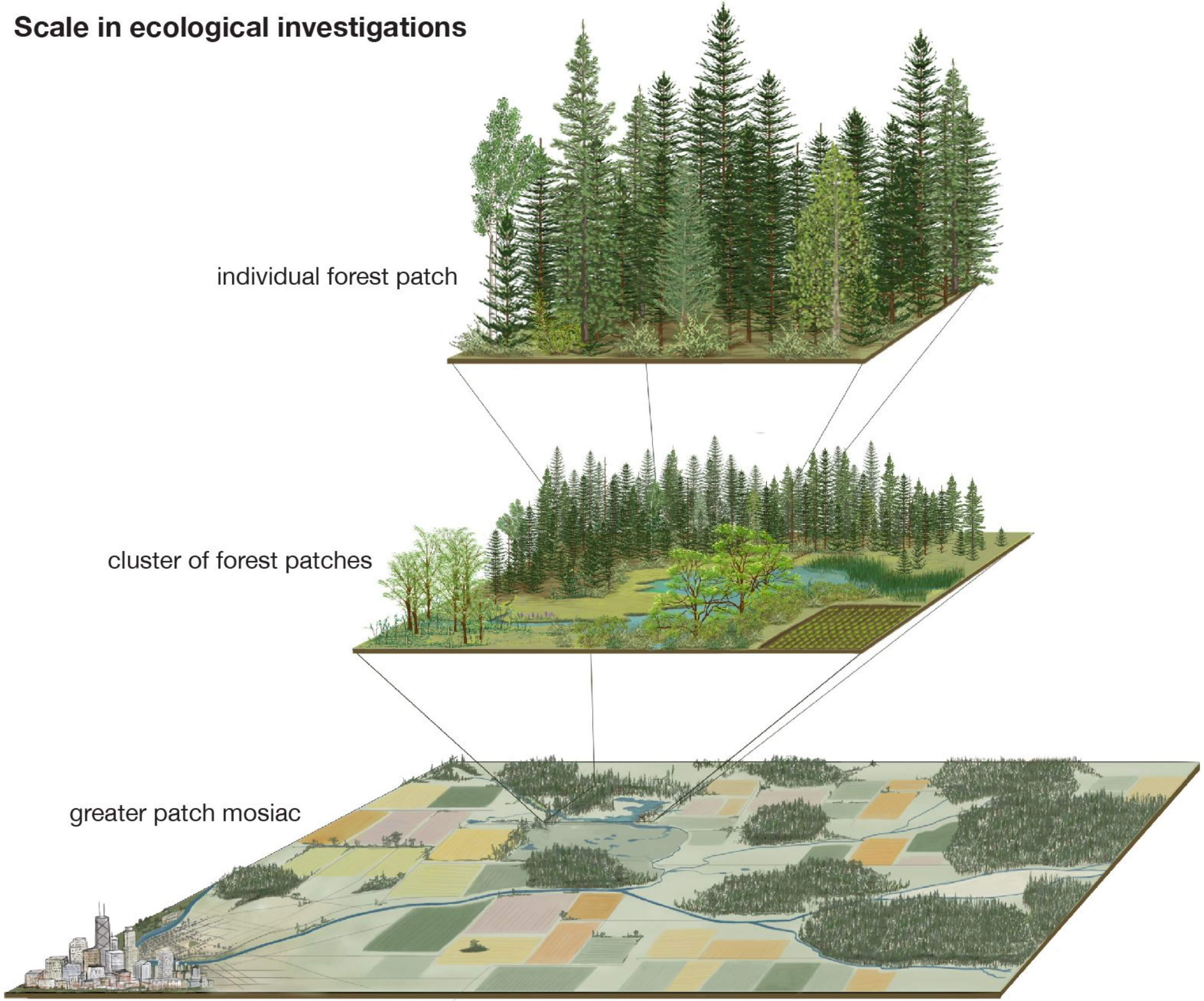
Individual processes can be represented by a multi-hypothesis approach, and ML provides an opportunity for a data-derived hypothesis that can be further explored or used to calibrate other hypotheses, when sufficient data are available.

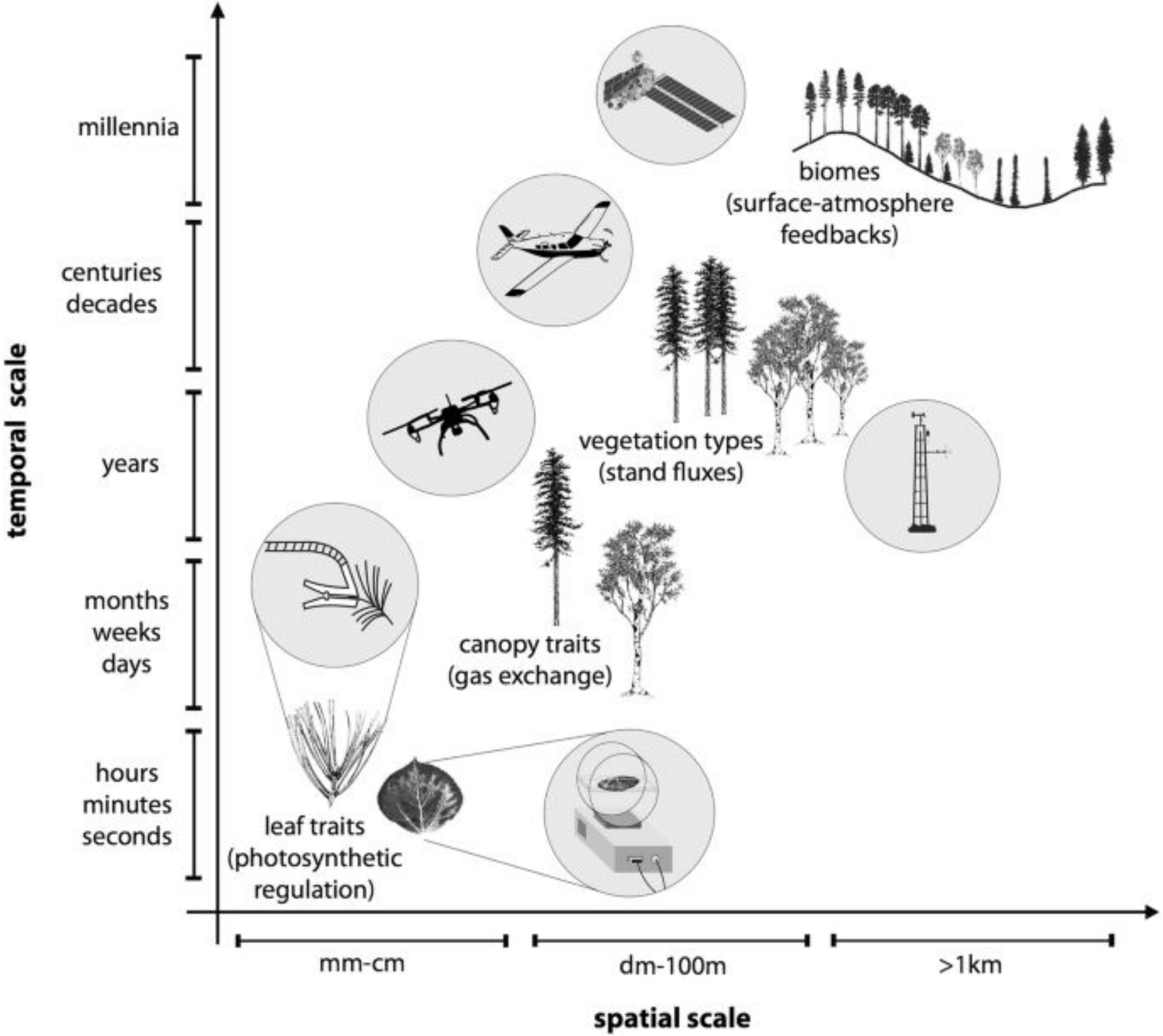


(a) Process Schematic of a Possible Full-Complexity Configuration of a Land Surface Model

(Fisher and Koven, 2020)

Scale in ecological investigations




temporal scale
millennia
centuries
decades
years
months
weeks
days
hours
minutes
seconds
biomes
(surface-atmosphere
feedbacks)
vegetation types
(stand fluxes)
canopy traits
(gas exchange)
leaf traits
(photosynthetic
regulation)
mm-cm
dm-100m
>1km
spatial scale

AI FOR SCIENCE TOWN HALL

Earth and Environmental Sciences

Forrest M. Hoffman (ORNL),
Rao Kotamarthi (ANL),
Haruko Wainwright (LBNL),
and the EES Writing Team

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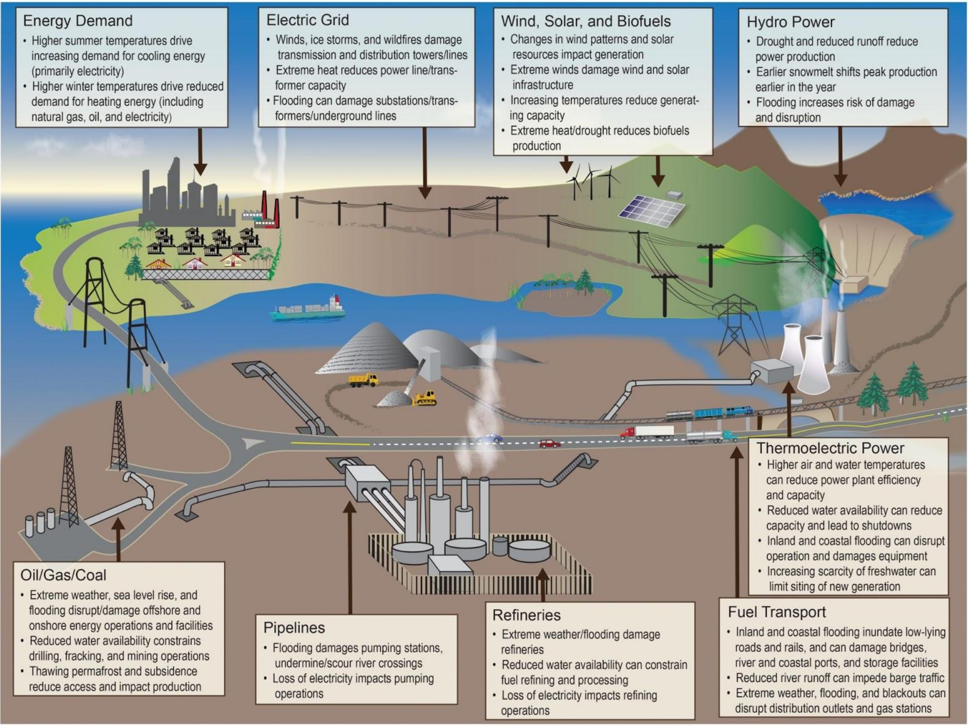
Grand Challenge #1



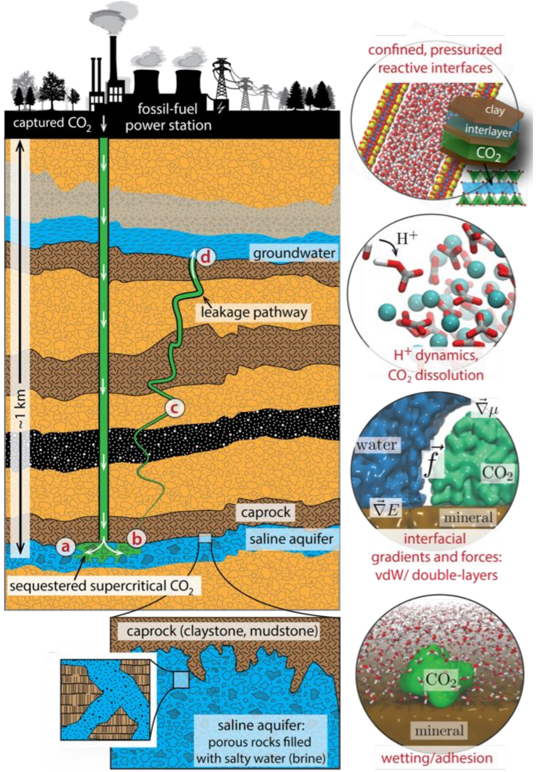
Project environmental risk and develop resiliency in a changing environment

- Increasing frequency of weather extremes and changing environment pose risks to energy infrastructure and the built environment
- Sparse observations and inadequate model fidelity limit the ability to identify vulnerability, mitigate risks, and respond to disasters

Grand Challenge #1

- New tools are needed to accelerate projection of weather extremes and impacts on energy infrastructure
- Building resiliency to address evolving risks will benefit from integration of smart sensing systems, built-for-purpose models, ensemble forecasts to quantify uncertainty, and dynamic decision support systems for critical infrastructure

Grand Challenge #2

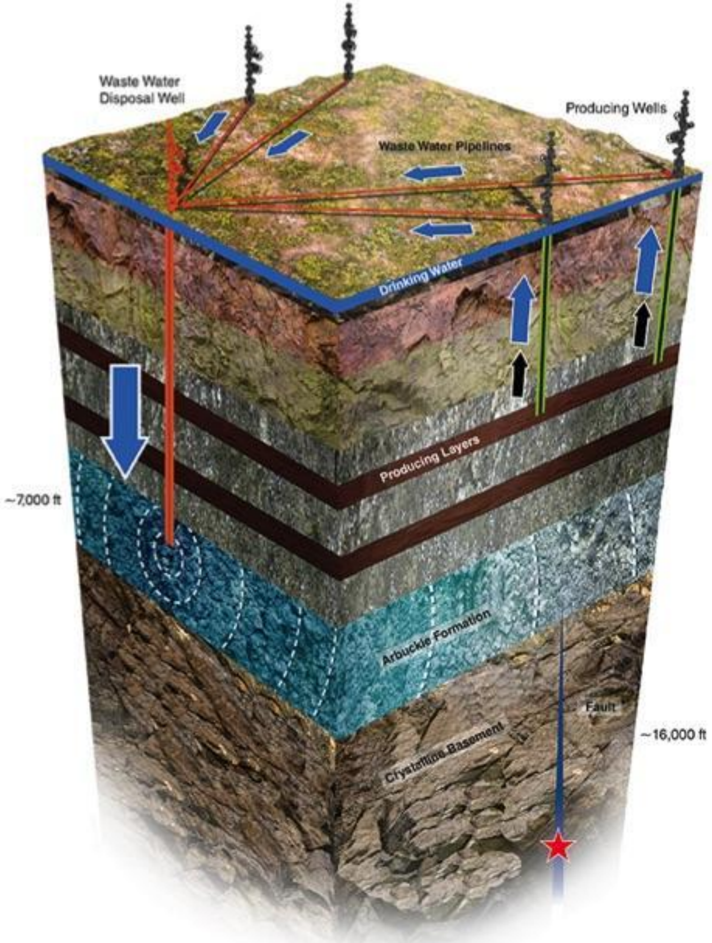


Characterize and modify subsurface conditions for responsible energy production, CO_2 storage, and contaminant remediation

- National energy security and transition to renewable energy resources relies on utilization of subsurface reservoirs for energy production, carbon storage, and spent nuclear fuel storage
- Subsurface data are uncertain, disparate, diverse, sparse, and affected by scaling issues
- Subsurface process models are incomplete, uncertain, and frequently unreliable for prediction

Grand Challenge #2

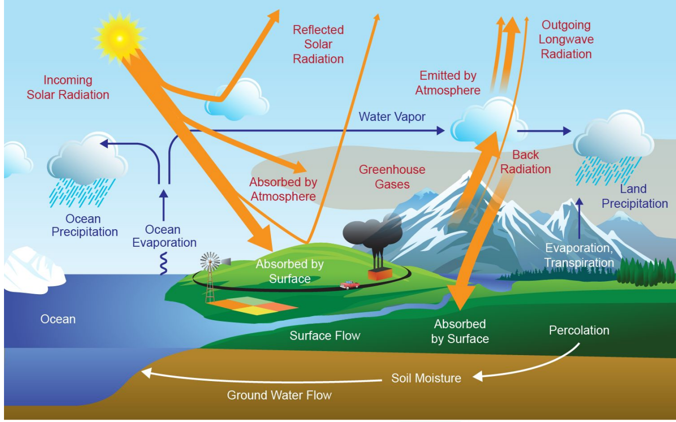
- We need to substantially increase hydrocarbon extraction efficiency, discover and exploit hidden geothermal resources, reduce induced seismicity and other impacts, improve geologic CO_2 storage, and predict long-term fate and transport of contaminants
- Mitigating risks requires improved subsurface characterization and assimilation of real-time data streams into predictive models of geological and ecological processes



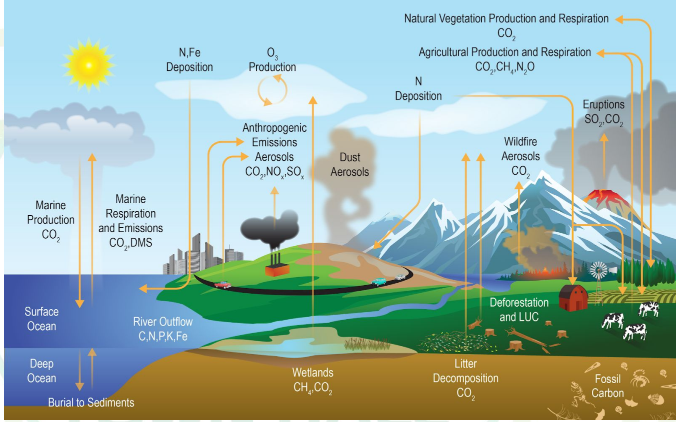
Grand Challenge #3

Develop a predictive understanding of the Earth system under a changing environment

- To advance the nation's energy and infrastructure security, a foundational scientific understanding of complex and dynamic hydrological, biological, and geochemical processes and their interactions is required (across atmosphere, ocean, land, ice)
- Knowledge must be incorporated into Earth system models to project future climate conditions for various scenarios of population, socioeconomics, and energy production and use



Energy & Water Cycles

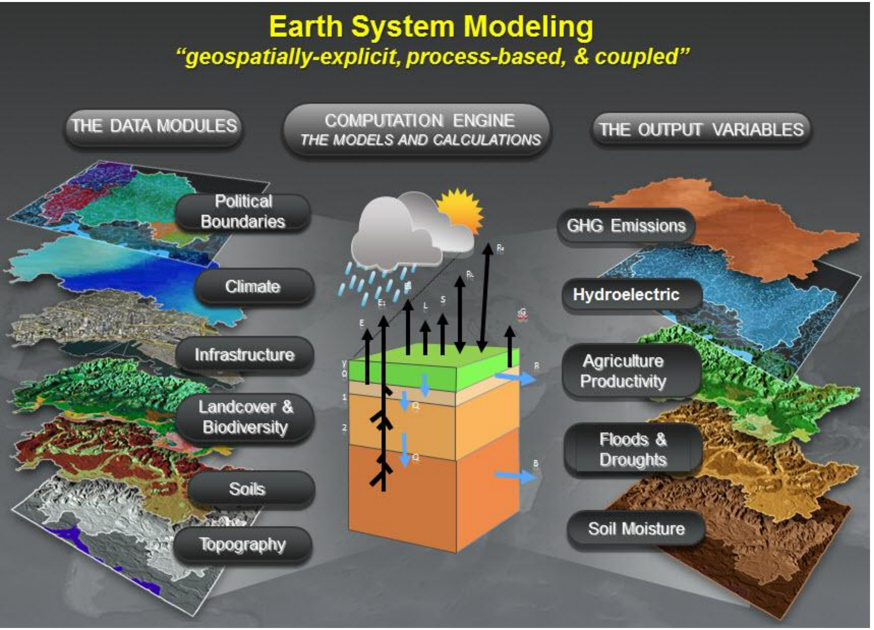


Carbon & Biogeochemical Cycles

U.S. DEPARTMENT OF ENERGY | Office of Science

Washington DC Town Hall
October 22-23

Grand Challenge #3

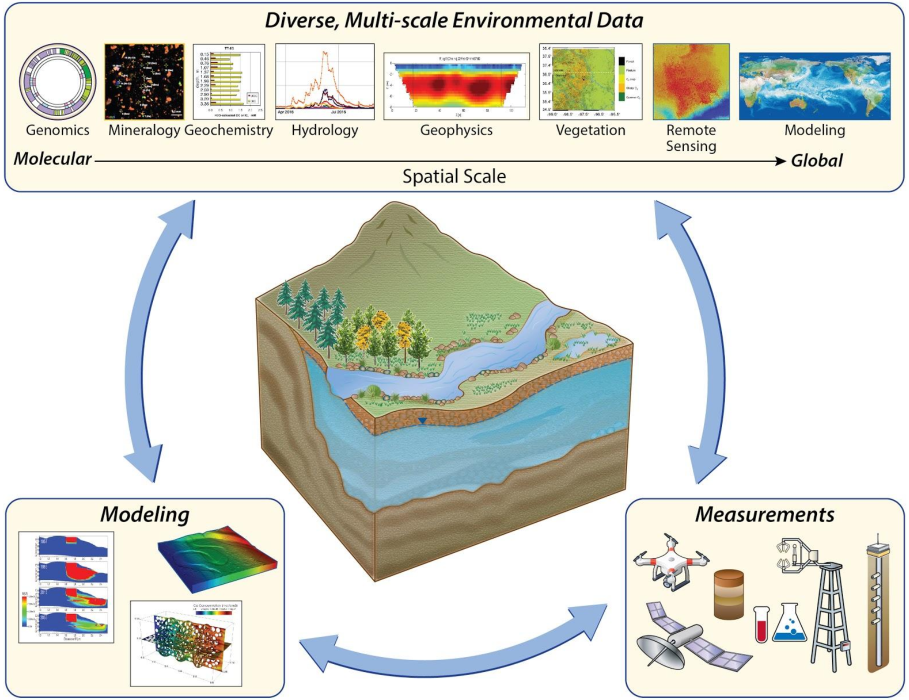


- Accurate predictions are needed to quantify changes in atmospheric and ocean circulation and weather extremes, to close the carbon cycle, and to understand responses and feedbacks of human, terrestrial, and marine ecosystems to environmental change
- Advances in genomics and bioscience data need to be leveraged to provide detailed understanding of plant–microbial interactions and their adaptations and feedbacks to the changing environment

Grand Challenge #4

Ensure global water security under a changing environment

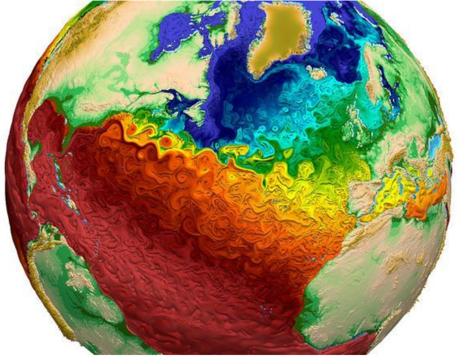
- Water resources are critical for energy production, human health, food security, and economic prosperity
- Water availability and water quality are impacted by environmental change, weather extremes, and disturbances such as wildfire and land use change



Grand Challenge #4

- Methods are needed to integrate disparate and diverse multi-scale data with models of watersheds, rivers, and water utility infrastructure
- Predictions of water quality and quantity require data-driven models and smart sensing systems
- Water resource management must account for changes in weather extremes, population, and economic growth

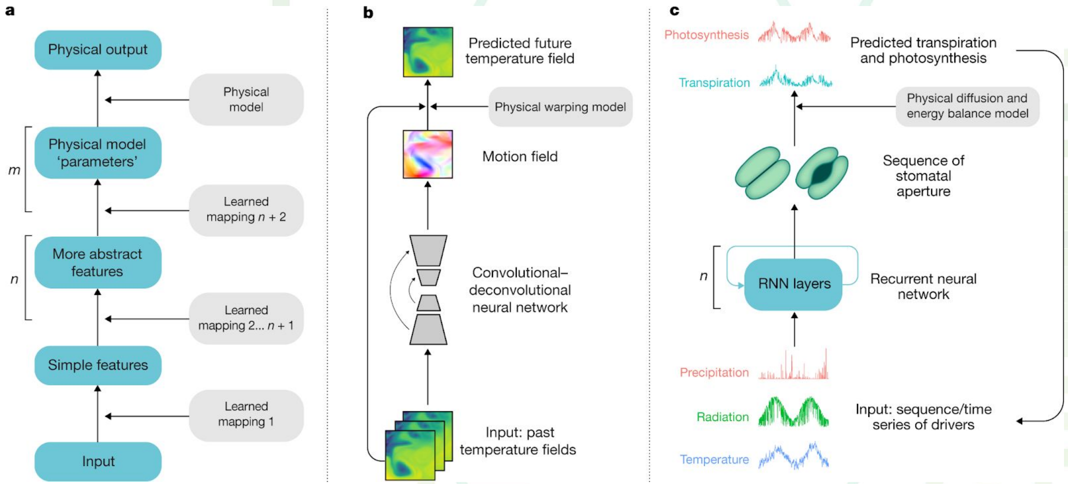
Accelerating Development



The near-term (5–10 years) priorities are to:

- Develop hybrid process-based/AI modeling frameworks for Exascale systems
- Develop strategies for mapping hybrid components on GPU/CPU based on computational density and communications patterns
- Develop physics / chemistry / biology-constrained ML
- Develop explainable AI and ML methods for hypothesis generation and testing

Hybrid Approaches to Earth Science Simulation (Reichstein et al., 2019)



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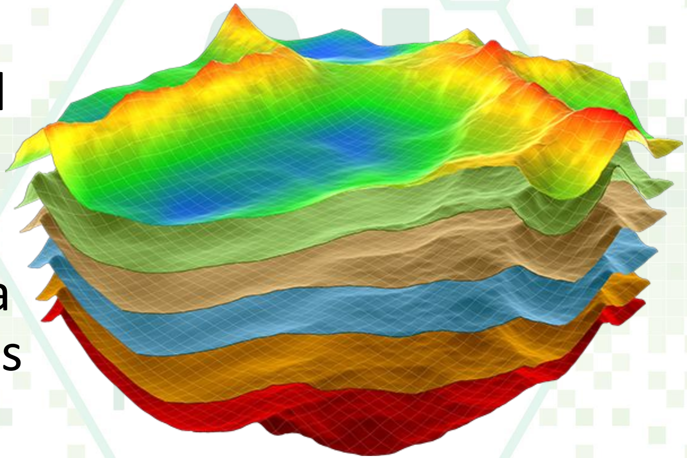
Expected Outcomes

- Model testbeds and surrogate models are expected to yield insights into process understanding across all Grand Challenges
- Data-driven and physics-constrained hybrid models are expected to stimulate new discovery and bridge space and time scales
- Integrated models of Earth system processes and energy/built infrastructure will enhance national energy and water security through simulation
- AI methods will enable effective use of large data streams for energy production, predictive process understanding, and environmental resiliency



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 a workshop in Fall 2021.

AI4ESP Workshop: Oct 25–Dec 3, 2021

Earth System Predictability Sessions

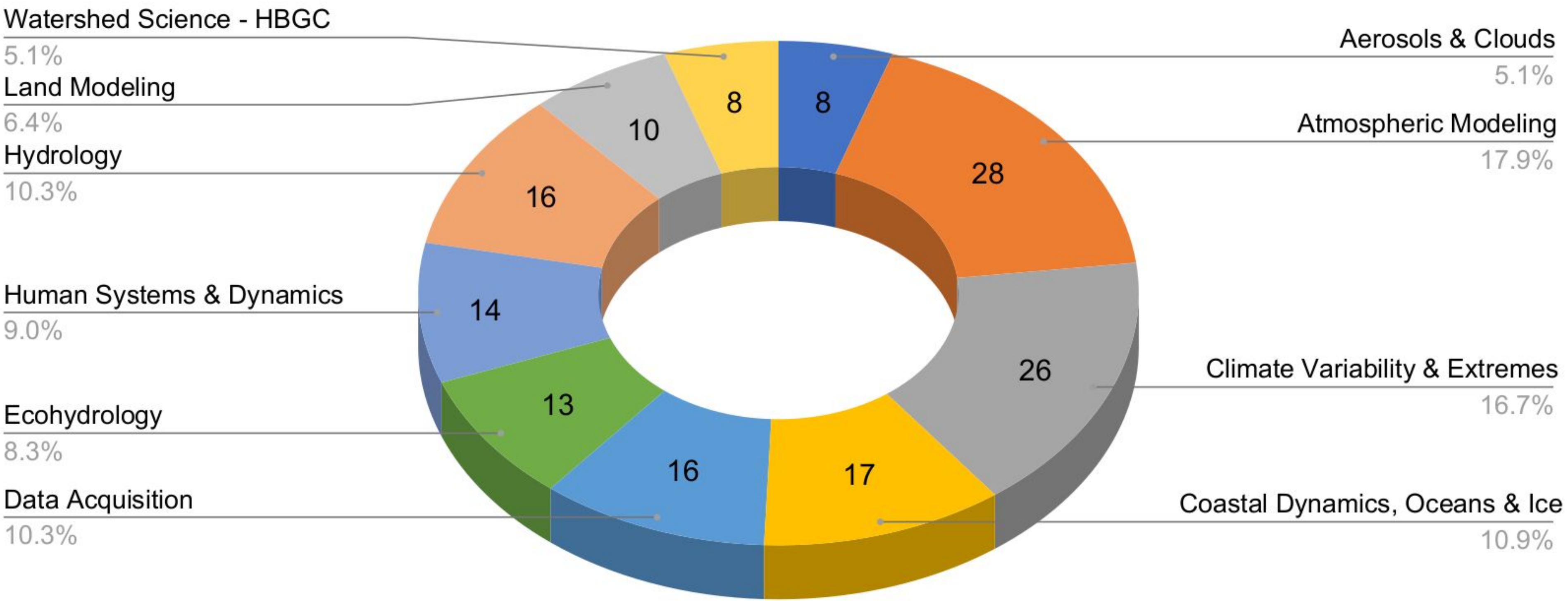
- Atmospheric Modeling
- Land Modeling
- Human Systems & Dynamics
- Hydrology
- Watershed Science
- Ecohydrology
- Aerosols & Clouds
- Climate Variability & Extremes
- Coastal Dynamics, Oceans & Ice

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

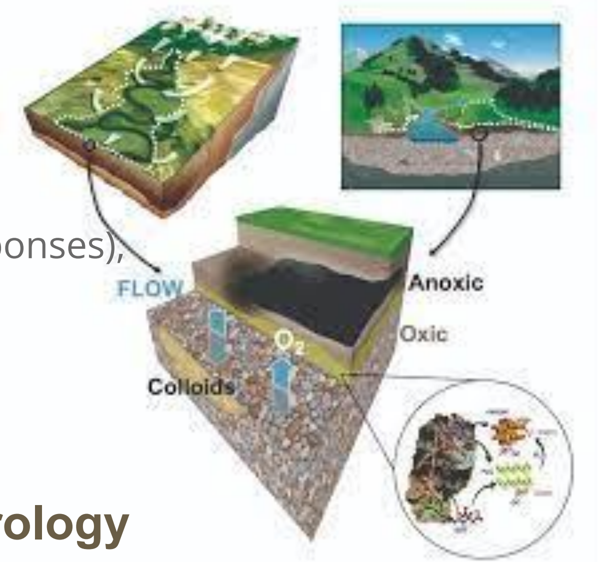
AI4ESP White Papers: Earth System Predictability Topics

Earth System Predictability Topics from 156 White Papers

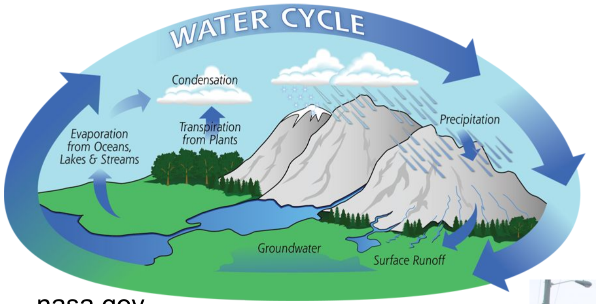


AI4ESP White Papers: Earth System Predictability Topics

- **Watershed science**
  - Hydro-Biogeochemistry, Soil biogeochemistry
  - Water quality
  - Lab-to-field, field-to-regional scale analysis
  - Experimental data, sensor networks (rapid responses), and experimental/network designs



ess.science.energy.gov



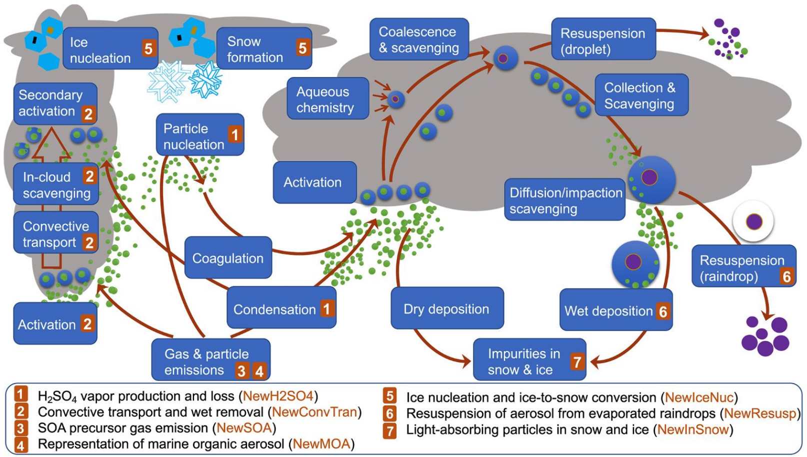
nasa.gov

climate.gov

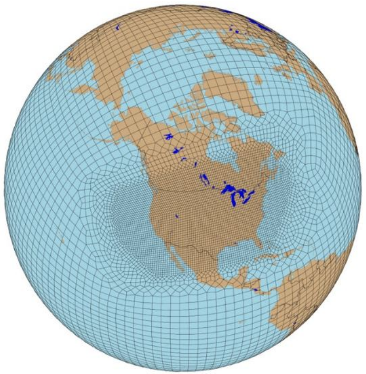
- **Hydrology**
  - Water resources
  - Precipitation-induced hazards (floods etc)
  - Weather/hydrological monitoring
  - Groundwater to surface water models
  - Mountain hydrology
  - Regional to continental scale

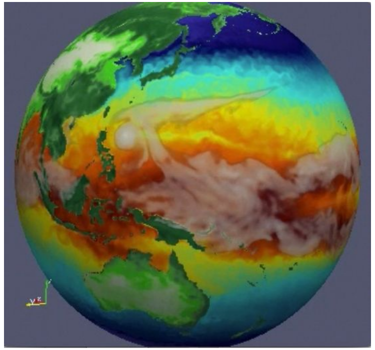
AI4ESP White Papers: Earth System Predictability Topics

- **Atmospheric Modeling**
  - Convection and turbulence
  - Surface Fluxes
  - Radiation
  - Model Tuning
  - General concepts that can generalized to other ESMs components



e3sm.org





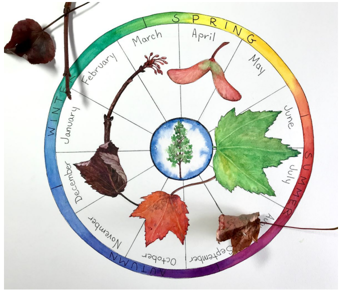
e3sm.org

- **Aerosols and Clouds**
  - Cloud Classification
  - Aerosol cloud interactions

AI4ESP White Papers: Earth System Predictability Topics

- **Land Modeling**
    - Agriculture / Crops
    - Leaf Phenology
    - Streamflow / Water Availability
    - Wildfire
    - Satellite Data Assimilation

Getty Images

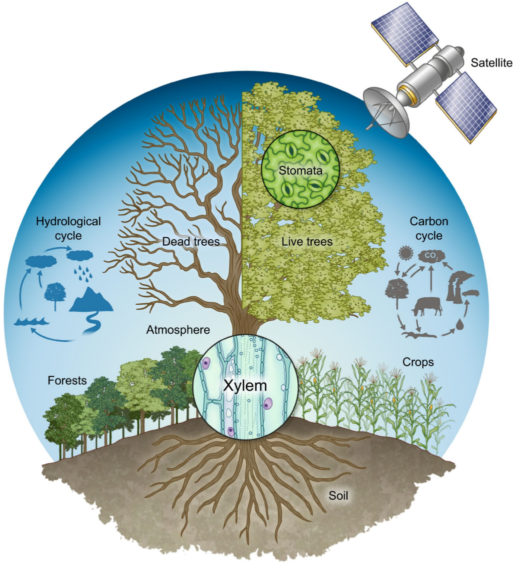


Adkins Arboretum

wallpaperbetter.com

- **Ecohydrology**
    - Stomatal Conductance / Photosynthesis
    - Plant Hydraulics and Growth
    - Evapotranspiration
    - Soil Moisture
    - Soil Hydrology

ABC7 News



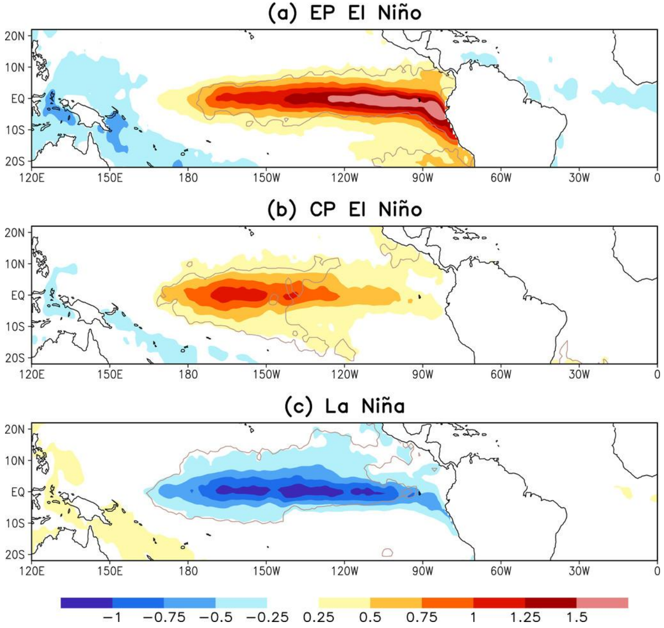
drought.gov

Nature

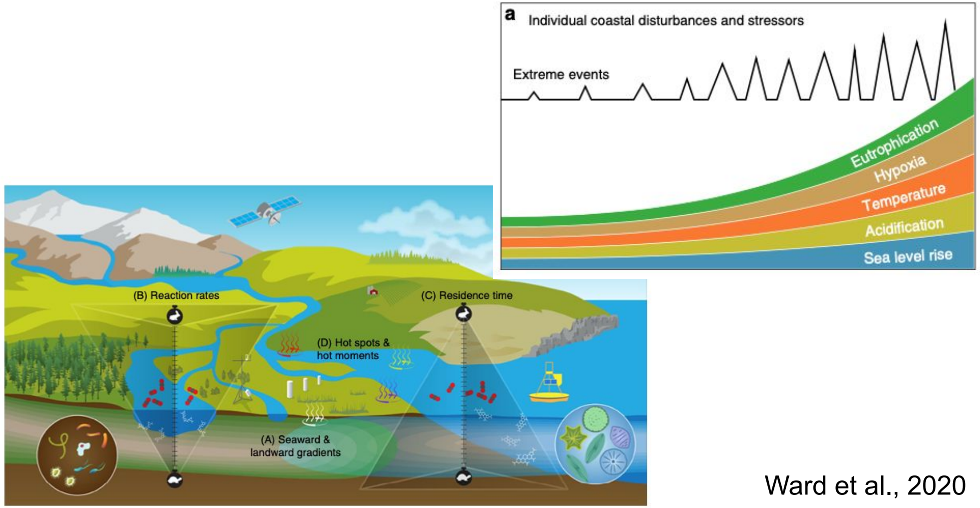
McDowell et al. (2019)

AI4ESP White Papers: Earth System Predictability Topics

- **Climate variability and Extremes**
  - TCs, ARs, Compound/Cascading events
  - Predictability
  - Circulation/climate variability (ENSO, NAO etc)
  - Telecommunication



Wang et al., 2014

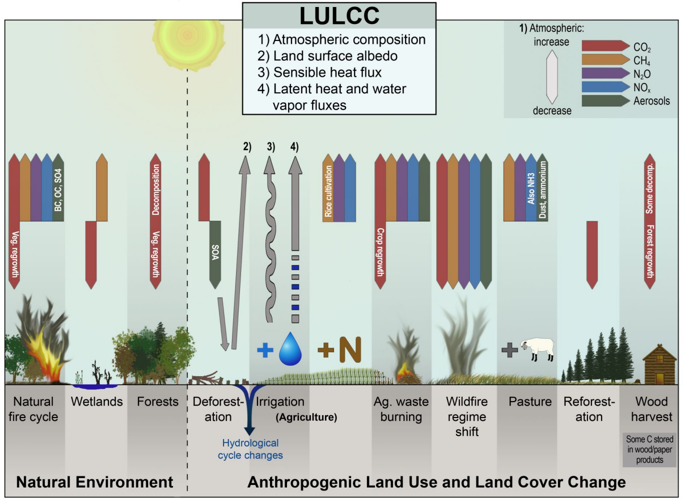


Ward et al., 2020

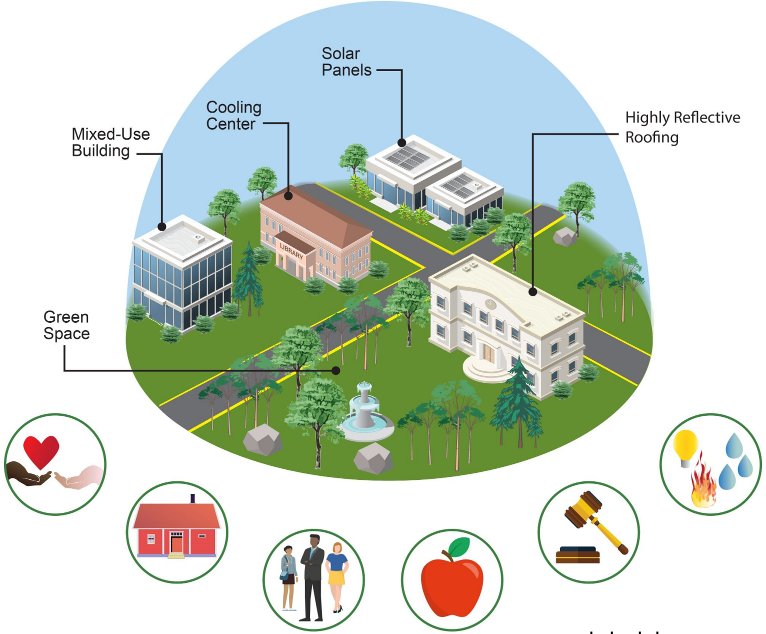
- **Coastal dynamics, Ocean/Ice**
  - Ocean/land/ice interface
  - Sea-level rise, storm surge
  - Coastal ecosystem/carbon cycling

AI4ESP White Papers: Earth System Predictability Topics

- **Human Systems and Dynamics**
  - Human activities/population
  - Energy-water-land nexus
  - Agriculture
  - Urban environment
  - Land use/cover changes



globalchange.gov



globalchange.gov

Workshop Agenda

WEEK 1		
North American Eastern Time	Day 1 **Monday, October 25, 2021**	Day 2 **Tuesday, October 26, 2021**
12:00	• Welcome - Nicki Hickmon • Deputy Secretary of Energy - David M. Turk • Introduction to AI4ESP Initiative - Nicki Hickmon • Earth & Environmental Systems Sciences Division (EESD) - Gary Geernaert • Advanced Scientific Computing Research (ASCR) - Barb Helland	Plenary Talk - Amy McGovern
12:15		Plenary Talk - Pierre Gentine
12:30		Break
12:45		Earth Science Topic Session **Land Modeling (Invited Only)** Session Chair: Beth Drewniak
13:15	**AI4ESP Workshop Structure, Charge & State-of-the-Science** AI4ESP Core Group: Nicki Hickmon, Haruko Wainwright, Forrest Hoffman, Scott Collis	
14:00	Break	
14:15	Panel Discussion Panel Chair: Rick Stevens Panel: Grace E. Kim, Prabhat Ram, Kirk Borne	
14:45		Break
15:00	Earth System Predictability Session **Atmospheric Modeling (Invited Only)** Session Chair: Ruby Leung	Cross-cut Session **Data Acquisition to Distribution (Invited Only)** Session Chair: Giri Prakash
17:00	Adjourn	Adjourn

WEEK 2		
North American Eastern Time	Day 3 **Monday, November 1, 2021**	Day 4 **Tuesday, November 2, 2021**
12:00	Reports from Previous Sessions (15 min) • Atmospheric Modeling • Land Modeling • Data Acquisition	Plenary Talk - Chaopeng Shen
12:15		Plenary Talk - Rob Ross
12:30	Break	Break
12:45	Earth Science Topic Session **Human Systems & Dynamics (Invited Only)** Session Chair: Christa Brelsford	Earth Science Topic Session **Watershed Science (Invited Only)** Session Chair: Mavrik Zavarin
14:45	Break	Break
15:00	Earth Science Topic Session **Hydrology (Invited Only)** Session Chair: Charuleka Varadharajan	Cross-cut Session **Neural Networks (Invited Only)** Session Chair: Nathan Hodas
17:00	Adjourn	Adjourn

WEEK 3		
North American Eastern Time	Day 5 **Monday, November 8, 2021**	Day 6 **Tuesday, November 9, 2021**
12:00	Reports from Previous Sessions (15 min) • Human Systems & Dynamics • Hydrology • Watershed Science • Neural Networks	Plenary Talk - Tapio Schneider
12:15		Plenary Talk - Alison Appling
12:30	Break	Break
12:45	Earth Science Session **Ecohydrology (Invited Only)** Session Chair: Forrest Hoffman	Earth Science Session **Aerosols & Clouds (Invited Only)** Session Chair: Po-Lun Ma
14:45	Break	Break
15:00	Cross-cut Session **Surrogate Models & Emulators (Invited Only)** Session Chair: Nathan Urban	Cross-cut Session **Knowledge-Informed Machine Learning (Invited Only)** Session Chair: Frank Alexander
17:00	Adjourn	Adjourn

WEEK 4		
North American Eastern Time	Day 7 **Monday, November 29, 2021**	Day 8 **Tuesday, November 30, 2021**
12:00	Reports from Previous Sessions • Ecohydrology • Surrogate Models and Emulators • Aerosols & Clouds • Knowledge-Informed Machine Learning	Plenary Talk - Laure Zanna
12:15		Plenary Talk - Katie Dagon
12:30	Break	Break
12:45	Earth Science Session **Coastal Dynamics, Oceans & Ice (Invited Only)** Session Chair: Matt Hoffman	Earth Science Topic Session **Climate Variability & Extremes (Invited Only)** Session Chair: Maria Molina
14:45	Break	Break
15:00	Cross-cut Session **Knowledge Discovery & Statistical Learning (Invited Only)** Session Chair: Xingyuan Chen	Cross-cut Session **Explainable/Interpretable/Trustworthy AI (Invited Only)** Session Chair: Line Pouchard
17:00	Adjourn	Adjourn

WEEK 5		
North American Eastern Time	Day 9 **Thursday, December 2, 2021**	Day 10 **Friday, December 3, 2021**
12:00	Reports from Previous Sessions • Coastal Dynamics, Oceans, & Ice • Knowledge Discovery & Statistical Learning • Climate Variability & Extremes • Explainable/Interpretable/Trustworthy AI	Reports From Previous Sessions • Hybrid Modeling • AI Architecture & CoDesign
12:15		Workshop session wrap-up and discussion motivation
12:30	Break	Break
12:45	Cross-cut Session **Hybrid Modeling (Invited Only)** Session Chair: Sivasankaran Rajamanickam	Panel/Open Discussion (Invited Only) **Common challenges & opportunities Resources, capabilities, and facilities** (DOE + Multi-agency)
14:45	Break	Break
15:00	Cross-cut Session **AI Architecture Co-Design (Invited Only)** Session Chair: Jim Ang	Panel/Open discussion (Invited Only) **Short-term, 5-year, 10-year goals Earth system predictability and applied math and computer science research priorities**
17:00	Adjourn	Adjourn

WEEK 6		
North American Eastern Time	Day 11 **December 7 or 8, 2021**	
12:00	Authors Meeting (Invited Only)	

- Public sessions (highlighted in green) are open to anyone; requires registration at https://ai4esp.org/workshop/
- Invitation-only sessions (highlighted in pink) are open to invited active participants and selected listening participants; requires registration on the Google Form link in the invitation email