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AI4ESP

ARTIFICIAL INTELLIGENCE FOR EARTH SYSTEM PREDICTABILITY

2021 WORKSHOP REPORT

Executive Summary

U.S. DEPARTMENT OF ENERGY

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Executive Summary

In October 2021, the U.S. Department of Energy (DOE) welcomed participants to the Artificial Intelligence for Earth System Predictability (AI4ESP) Workshop,[1] hosted by the Office of Biological and Environmental Research (BER)—Advanced Scientific Computing Research (ASCR). The workshop is part of BER-ASCR's ambition to more radically and aggressively advance prediction capabilities in the climate, Earth, and environmental sciences through the use of modern data analytics and artificial intelligence (AI). Advances in these capabilities are needed to improve predictions of climate change and extreme events that provide actionable information for planning and building resilience to their impacts.

A distinguishing aspect of this workshop was the framing around BER's "Model-Experimentation" (ModEx) integrative research process, which involves integrating observations, experiments, and measurements, performed in the field or laboratory, with model research that simulates these same processes. This iterative approach enables models to generate hypotheses that inform field and laboratory efforts to collect data, which are subsequently used to parameterize, drive, and test model predictions. Hence, this workshop was unique in seeking an immense breadth of AI applications to enhance Earth system ***models, observations, and theory,*** as well as the computational infrastructure and transdisciplinary collaborations that enable their seamless integration.

The scientific challenges framing these disciplines have become increasingly complex and beyond the reach of traditional approaches. Hence, BER and ASCR encouraged workshop attendees to be bold with out-of-the box thinking, even considering a paradigm shift in the approach to scientific discovery and enhanced predictability. Sessions were organized around nine Earth system predictability science topics and eight cross-cutting artificial intelligence/machine learning (AI/ML) topics (see *A Community-driven Workshop* below). All sessions included in-depth discussions of the following: (1) the grand challenges that must be tackled; (2) state-of-the-science; (3) opportunities to advance science using radical approaches; (4) research priorities; and (5) 2-, 5-, and 10-year goals to frame the community's engagement. This comprehensive report summarizes the major outcomes of the workshop with an overarching goal to define priorities that can yield the most impactful science.

A COMMUNITY-DRIVEN WORKSHOP

A total of 17 topics were addressed at the 2021 AI4ESP workshop sessions. These topics emerged from 156 white papers submitted from the community in response to BER-ASCR's call to develop AI methods and applications in BER research areas. The workshop sessions emphasized quantifying and improving Earth system predictability, particularly related to the integrative water cycle and associated water cycle extremes.

EARTH SYSTEM PREDICTABILITY SESSIONS

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

CROSS-CUT SESSIONS

- Data Acquisition to Distribution
- Neural Networks
- Surrogate Models and Emulators
- Knowledge-Informed Machine Learning
- Knowledge Discovery and Statistical Learning
- Explainable/Interpretable/Trustworthy AI
- Hybrid Modeling
- AI Architectures and Co-design

1 See https://www.ai4esp.org and https://www.ai4esp.org/workshop/.

AI-enabled Earth System Science: Pressing Need for Paradigm Change

AI technologies have expanded exponentially over the past decade and are well positioned to accelerate predictions of Earth system processes. The current paradigm governing scientific discovery is that process understanding derived from measurements underpins our ability to create models that make predictions and long-term projections. However, the progress in physical understanding often does not transfer to actionable predictions due to the complexities associated with chaotic interacting components of Earth systems. Challenges include the wide range of relevant scales (microbe-to-global spatial scales, minutes-to-centuries temporal scales), the nonlinear interactions of multi-scale processes and human impacts, and the outsized impacts of extreme events on the environment.

Scientists and stakeholders are increasingly demanding predictions that have finer resolution, larger spatial domains, greater accuracy, and longer time horizons. Some examples include an urgent need for more accurate prediction of extreme events and their impacts, enhanced understanding of processes and strategies to make natural and human systems more resilient to climate change, and more complete characterization of uncertainty and biases in models and data to constrain scientific findings. While the increase in supercomputing capacity has allowed finer scales to be explicitly resolved in process-based models, achieving high-resolution simulations across large spatial domains is still beyond current capabilities for many models, especially when large ensemble runs and new process representations are needed to improve accuracies.

AI technologies—neural networks, classical machine learning models, optimized data acquisition and assimilation, computer vision, and unsupervised and reinforcement learning techniques—are tools that must be harnessed to accelerate progress in Earth system observations and models. The challenges to increase resolution and process fidelity and reduce the uncertainty of Earth system predictions require novel approaches that assimilate AI into traditional experiments, models, and data acquisition methodologies. This hybridized approach, while attractive, leads to new challenges, such as developing massive multi-scale datasets that require new AI techniques to understand cause and effect; overcoming huge computational costs where intelligent sensitivity analysis and uncertainty quantification must make progress; and requiring new parameterizations of important nonlinear scales that bridge the natural and human components in complex systems such as those found in urban regions.

The AI4ESP vision aims to dramatically accelerate Earth system models, observations, and theory by taking advantage of rapid progress in machine learning methodologies in conjunction with advances in big data infrastructure, analytics, optimized hardware architectures, networking and edge computing technologies, and other computational tools that were unavailable even a decade ago (Figure ES-1). This vision requires co-design and co-investment in observational capabilities and platforms, models and software infrastructure, and computational hardware to develop AI approaches specifically aimed at the climate, Earth, and environmental system sciences. Notably, this goes beyond AI technologies that to date have benefitted from massive investment in the private sector as they are optimized for commercial applications. Although there are opportunities to apply commercial AI tools for Earth system predictions, new scientific AI methodologies that incorporate process understanding and respect physical laws are required to make Earth system models interpretable, trustworthy, and robust.

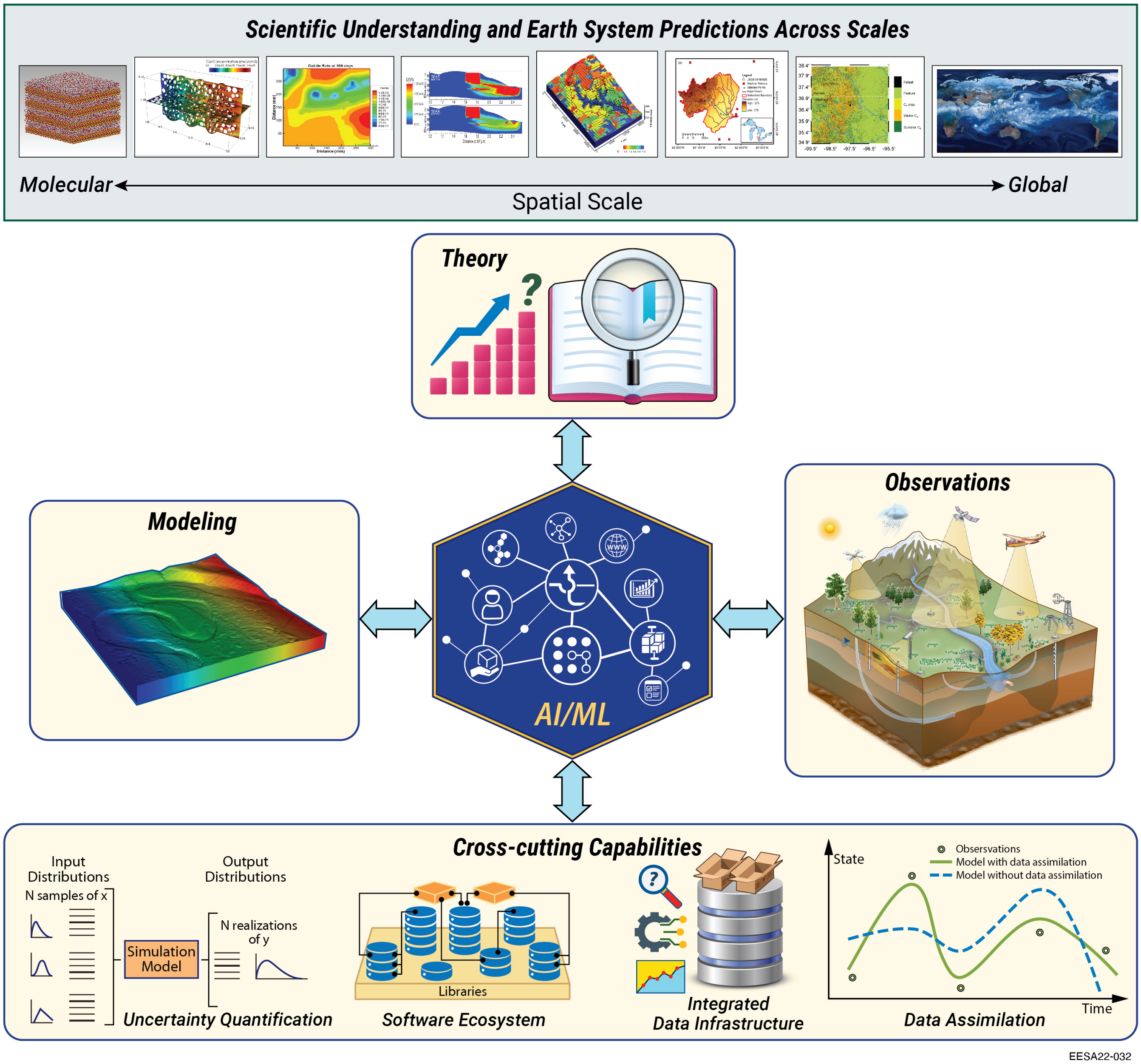

Figure ES-1. Conceptual diagram showing how Artificial Intelligence and Machine Learning (AI/ML) can enhance and be informed by the three pillars of Earth sciences—observations, modeling, and theory—as well as cross-cutting computational capabilities. The integrated outcomes from modeling, experimentation, and theoretical knowledge generation will enhance the scientific understanding and predictions of Earth systems processes across multiple spatial scales (Source: Lawrence Berkeley National Laboratory 2022).

Background of AI4ESP

AI4ESP began as a multi-laboratory collaboration within the DOE, which brought the labs together to understand the key challenges and opportunities in AI/ML methods. The goal is to radically improve predictive capabilities by determining the most impactful AI/ML applications that span the continuum from observations to multiscale modeling and analysis.

Planning for AI4ESP was initiated by scientists from three DOE national labs with leadership-class computing facilities—Argonne National Laboratory, Lawrence Berkeley National Laboratory, and Oak Ridge National Laboratory. However, the planning team rapidly expanded to engage scientists from five additional national laboratories: Brookhaven National Laboratory, Los Alamos National Laboratory, Lawrence Livermore National Laboratory, Pacific Northwest National Laboratory, and Sandia National Laboratories.

These scientists recognized the importance of broad participation and reached out to the Earth sciences, computing, and AI communities throughout the private and public international research enterprise through a white paper call. This outreach resulted in an encouraging response of 156 white papers[2] from 640 unique authors across 112 unique institutions. Based on this response, AI4ESP leadership brought together a diverse group of approximately 100 people to design a workshop that would offer an open, collaborative environment to listen to and share ideas for understanding the opportunities for a paradigm shift in incorporating AI as a component of Earth system models and observations. This effort resulted in a virtual workshop, spanning five non-consecutive weeks in late October through early December of 2021 that engaged participants with diverse expertise across Earth and environmental sciences, computational sciences, and engineering (see *Workshop Participants* box).

WORKSHOP PARTICIPATION

The 156 white papers were from 640 unique authors across 112 unique institutions. AI4ESP leadership brought together 100 researchers to design the virtual workshop, which:

- Spanned five non-consecutive weeks from October–December 2021.
- Engaged more than 740 participants from 178 institutions.
- Of the participants, 83% were domestic and 17% were international.

Workshop Outcomes: Three Priorities

The AI4ESP workshop resulted in multiple overarching themes with recurring and common challenges, needs, and opportunities across many sessions. From these, three major categories of priorities emerged: (1) *Earth science,* (2) *computational science and methodology,* and (3) *programmatic and cultural changes to achieve a multidisciplinary and unified framework.* In particular, the workshop emphasized the need to incorporate AI into models, analytics, and data generation as a means to accelerate advancement, create new scientific opportunities, and revolutionize new approaches to predictive capabilities and capacity. The 2-, 5-, and 10-year priorities (Figure ES-2) identified across each of the workshop sessions could provide the basis for a roadmap to achieving the AI4ESP vision (Figure ES-3).

2 See https://www.ai4esp.org/white-papers/.

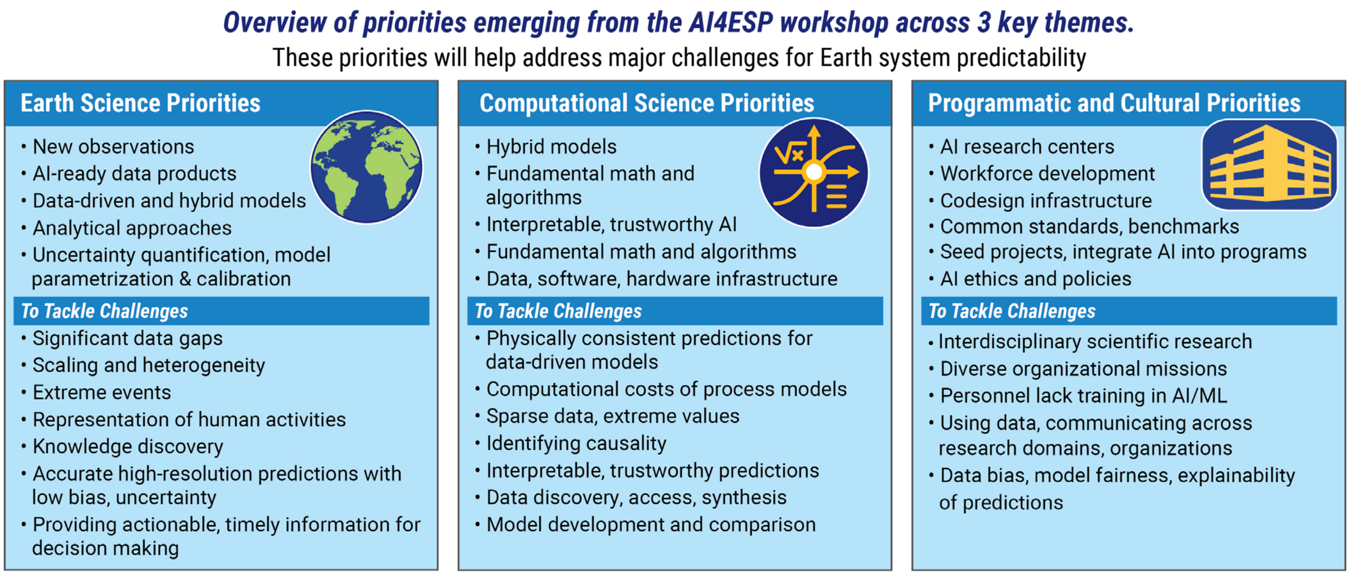

Figure ES-2: The AI4ESP workshop participants identified grand challenges and 2-, 5-, and 10- year research priorities to advance the use of AI/ML in Earth systems science. Several common themes emerged across the 17 sessions that fell broadly under the categories of Earth sciences, computational sciences, and programmatic and cultural changes to achieve a multidisciplinary framework (Source: Lawrence Berkeley National Laboratory 2022).

Earth Science Priorities

Some common challenges emerged from the various workshop discussions that involved Earth science topics. In general, the discussions all emphasized the central challenge of making dramatically improved predictions and observations across a wide range of spatial and temporal scales, and doing so with sufficient resolution and accuracy to be of use to decision-makers and scientists. Several other challenges would need to be addressed to accomplish this goal, which include (1) capturing heterogeneity in the relevant variables and processes, (2) overcoming the difficulty associated with observing and predicting extreme events, (3) managing and analyzing the immense volumes of data across a variety of ecosystems, and (4) launching a major effort to identify robust, interdisciplinary scientific approaches that integrate human activities.

The Earth system priorities focus on opportunities where AI can help address these challenges and reduce uncertainties. These included priorities for:

- ☐ Advancing scientific understanding and knowledge discovery
- ☐ Developing approaches for obtaining new measurements at desired scales and resolutions
- ☐ Prioritizing the collection, synthesis, and curation of data most valuable for advancing AI in different Earth science domains
- ☐ Creating AI-ready datasets, such as standardized benchmarks, and quality-checked and gap-filled data for model training, verification, and validation
- ☐ Incorporating AI/ML into Earth system models (e.g., surrogate models, emulators, and hybrid ML-/process-based models) to help address challenges related to scaling and process heterogeneity for accurate, high-resolution predictions with reduced bias and quantified uncertainties
- ☐ Improving predictive capabilities of extreme events and ecosystem disturbances including compounding events (e.g., coincident heat waves and droughts) and cascading impacts, given sparse data and lack of prior event analogs

- Improving representation of human-driven processes and interactions in models
- Quantifying the impact of all sources of error and uncertainties (e.g., arising from unknown model parameters, noisy data, missing processes, discretization errors in the solution of model equations, and approximations in reduced-order models or ML models)
- Developing a systematic framework, metrics, and workflows for model training, calibration and optimization, verification and validation, and intercomparison
- Employing AI/ML to provide the scientific foundations and identifying critical pieces of information to support decision-making at various scales

Computational Priorities

Common computational challenges that emerged across the sessions include the development of: (1) large, curated datasets for model training; (2) new mathematical approaches tailored for sparse data and extreme events; (3) novel approaches that address interpretability and potential physical inconsistencies of traditional ML model outcomes, driving the need for hybrid models; (4) innovative and consistent approaches to represent model uncertainties and trustworthiness; (5) software infrastructure for supporting hybrid model components across major Earth and environmental system science codes; and (6) efficient and interoperable frameworks and architectures that provide access to data and model resources across organizations.

The computational priorities identified future developments and advancements in AI and ML techniques, algorithms, mathematical frameworks, data management, tools and libraries, and hardware architectures, including for:

- Developing portable and efficient software infrastructure for systematically combining traditional process parameterizations with data-driven models for hybrid modeling and data assimilation, supporting plug-and-play parameterization swapping and online training
- Advancing fundamental math and algorithms for working with complex systems, sparse data, long system memory, and extreme values
- Developing methods to extract causal relationships and mechanisms and to offer robust interpretability and explainability of the ML model outcomes toward application-specific, explainable, and interpretable AI
- Developing AI-guided data acquisition frameworks that leverage adaptive observational capabilities such as edge computing and autonomous instrumentation, and that inform optimal data collection strategies
- Co-designing computational and storage infrastructure for automated ML model selection, design and training, integration of process and ML models, model intercomparison, and data assimilation
- Developing AI-assisted data discovery and synthesis, scientific data management archives, and tools that provide efficient access to and use of data across organizations and computational resources

A Unified Framework to Incorporate Multidisciplinary Priorities and Cultural Change

Numerous programmatic and cultural needs were identified across all sessions, which include the need for (1) bridging multi-domain and multi-mission demands across different science and government communities; (2) having a trained workforce capable of interdisciplinary research across Earth and computational sciences; and (3) coordinating data generation, standards, synthesis, and model development efforts across different research groups. Development of a supporting framework to bridge these community-wide barriers would allow current and future activities to efficiently collaborate and accelerate development of AI research and technologies. In particular, *workshop participants clearly signaled the need to create a radically different approach for future AI-enabled Earth system modeling and observational efforts that will enable and foster collaborations across disciplines and institutions.* Notably, AI4ESP's focus on BER's ModEx approach, namely, using AI to enhance models, observations, and theory (Figure ES-1), makes the priorities identified by the AI4ESP community unique to the DOE scientific mission.

Workshop participants clearly signaled the need to create a radically different approach for future AI-enabled Earth system modeling and observational efforts that will enable and foster collaborations across disciplines and institutions.

Achieving the AI4ESP vision will require an unprecedented level of coordination across scientific disciplines and public, private, government, and scientific communities. Priorities identified to address these barriers include:

- Creating AI research centers tasked to coordinate and collaborate to more rapidly advance priorities across the various Earth science topics, where the centers would provide the supporting data and computational infrastructure, mathematical capabilities, and cross-disciplinary expertise to support community ambitions
- Co-designing frameworks or platforms to enable communities with different missions to efficiently share applicable results, techniques, data, and codes to decrease unnecessary duplication of effort and accelerate the application of AI
- Determining cross-disciplinary data-sharing standards, and creating shareable benchmark and training datasets that bridge organizations
- Supporting working group activities to investigate major and timely transdisciplinary research questions and quickly enhance or test developments such as workshops, challenges, and hackathons through a center or facility that is staffed to support commonly used data, models, and workflows
- Developing standards for trustworthy AI, including addressing data biases, ensuring fairness in models, and fostering the ethical and responsible development and use of AI
- Building public-private partnerships that enable use of commercial tools for research purposes and vice versa
- Focusing on new efforts to inspire and motivate the next-generation workforce, including training of multidisciplinary scientists, as well as outreach to a broader and more diverse set of academic and laboratory institutions
- Supporting early success stories to support training, inspiration, and strategic program design, such as through demonstration projects, infusion of AI into existing funded programs, and follow-up "implementation workshops" on key topics to chart roadmaps

Beyond the AI4ESP Workshop

The success stories that are highlighted in this report and outcomes from the workshop deliberations clearly point to the potential for AI/ML to accelerate integrated, next-generation observations and models that incorporate complex natural and human processes at sufficient resolutions to support emerging science challenges, as well as to improve decision-making. There was broad consensus that AI can be transformational and help address long-standing grand challenges in Earth and environmental sciences, but that significant research and development in both AI and domain sciences are needed for this to happen.

Since completion of the workshop, participants have continued both high-level and specific topical discussions at conferences, such as the American Geophysical Union (AGU) 2021 Fall Meeting and the American Meteorological Society (AMS) 2022 Annual Meeting. Participants have also carried forward the information from the AI4ESP workshop to other community activities, including the SIAM AI4ESP workshop summary, National Academies Machine Learning and Artificial Intelligence to Advance Earth System Science workshop, and an upcoming special collection of the American Meteorological Society AI for Earth Systems (AIES)[3] journal to promote information distribution from the workshop. Related workshops and meetings are expected in the future to capitalize on new collaborations and develop the underlying building blocks needed to develop a community-wide framework.

REPORT ORGANIZATION

The full report is designed to provide additional levels of detail in the following sections. The Workshop Summary provides references to past and ongoing activities, examples of AI applications involving Earth science, and both opportunities and research priorities identified across the 17 sessions. Individual chapter reports follow that dive into each of the Earth science domains and the AI/ML session topics. Finally, the appendices contain acronyms (Appendix A), the workshop agenda (Appendix B), call for white papers (Appendix C), lists of participants (Appendix D), and list of white papers (Appendix E).

A link to the full PDF report can be obtained here.[4]

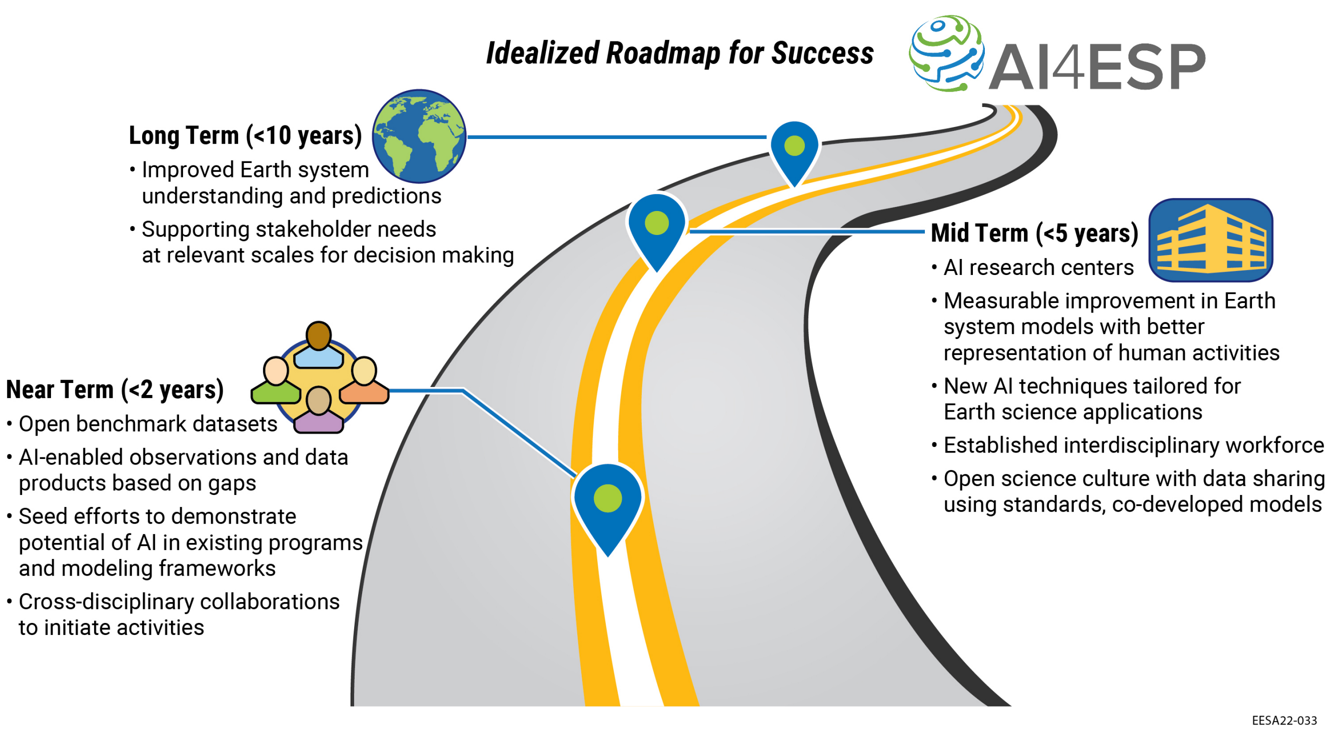

Figure ES-3: Roadmap to the execution of AI4ESP encompassing near- (2-year), mid- (5-year), and long-term (10-year) activities (Source: Lawrence Berkeley National Laboratory 2022).

3 See, respectively, https://sinews.siam.org/Details-Page/improving-earth-system-predictability-with-artificial-intelligence; https://nap.nationalacademies.org/catalog/26566/machine-learning-and-artificial-intelligence-to-advance-earth-system-science; and https://www.ametsoc.org/index.cfm/ams/publications/journals/artificial-intelligence-for-the-earth-systems/.

4 See https://ai4esp.org/.

AI4ESP

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.

The Artificial Intelligence for Earth System Predictability initiative is a collaboration between the U.S. Department of Energy management and laboratories to understand the paradigm shift required to enable artificial intelligence across the ModEx enterprise, in part by determining the most impactful applications along the observation-modeling continuum.

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