Emergent Concepts from a Community Ideation on AI4ESP

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This AI4ESP white paper is the outcome of an open ideation session led by PNNL that numerous institutions participated in. The leadership team included Amy Goldman, Huiying Ren, Tim Scheibe, and James Stegen. The white paper is broken into two sections: (1) A summary of the ideation session, and (2) a short summary of a 'meta idea' that emerged from combining multiple ideas spanning the three primary focal area themes articulated in BER's AI4ESP guidance: A - Data Acquisition and Assimilation, B - Predictive Modeling, and C - Insight from Complex Data. The white paper, therefore, has two goals. The first section is meant to be a resource for innovating around how to pursue open, community-based ideation in virtual environments. The second section is meant as an example of the kinds of 'meta ideas' that can emerge from bringing diverse ideas together in a single shared space. We consider the second section to be a submission to BER's request for white papers around AI4ESP.

Section 1: Summary of the community ideation session

Motivation and Goal. The integrated Earth system is changing due to disturbances from local to global scales, leading to a pressing need to dramatically improve our ability to predict future functional and structural states. To take a paradigm-shifting step forward requires more than a single person and more than a single team, hence BER's interest in AI4ESP white papers. Bringing ideas together in an open, dynamic ideation space can lead to outcomes that are more than the sum of individual ideas and single teams. We recognized a need for such an environment and, in turn, held an ideation session that was open to all interested in developing an AI4ESP white paper. The goal was to maximize advancement towards the AI4ESP goals, ultimately to benefit the broader science community and society.

Vision and Philosophy. The vision of the ideation session was simple: set up an environment that would facilitate creating, sharing, and integrating ideas while developing new conceptual and collegial connections, all of which may not have arisen otherwise. The PNNL leadership team's philosophy was to facilitate the community towards meeting BER's goals without the intention of PNNL necessarily taking ownership over the resulting ideas or white papers. All generated ideas and other materials are from the community and belong to the community, of which the PNNL leadership team is a part.

Approach. The ideation session was based on Kate Maher's "S^3" approach that progressively moves through **S**olo ideation, **S**haring the resulting ideas in a small group, and **S**ynthesizing ideas through within and cross-group interactions. This "S^3" approach has been used in multiple BER-focused group environments with great success as it overcomes many of the traditional issues with group brainstorming. For example, it allows space and opportunity for more voices and ideas that would be hard otherwise. This is essential given BER's goal of developing truly transformative ideas to improve Earth system predictions.

In the case of this ideation session, the "S^3" approach was used to develop ideas that participants could rally around to develop whitepapers. Doing so required a very dynamic environment that went from the whole 100+ person group, to small groups and solo work, back to the whole group, breaking into new small groups, and back to the whole group. Doing this in a virtual environment necessitated the use of several technologies combined in a novel way.

The opening plenary kickstarted in the Microsoft (MS) Teams platform to highlight whitepaper themes and introduce this ideation session structure to the attendees. Attendees

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were then instructed to enter Gather.Town, a website (https://gather.town/) that allows for voice/video communication embedded in a 2D graphical interface wherein each attendee is reflected by an avatar that moves freely around in a virtual conference center space. The virtual space was customized by the ideation session leadership team to accommodate the specific needs of this effort. In Gather.Town, attendees' avatars joined one of three rooms based on the guiding focal areas described in the white paper call. Each room was supported by a facilitator, and attendees moved their avatar into small breakout groups within these rooms for ideation activities (Figure 1).

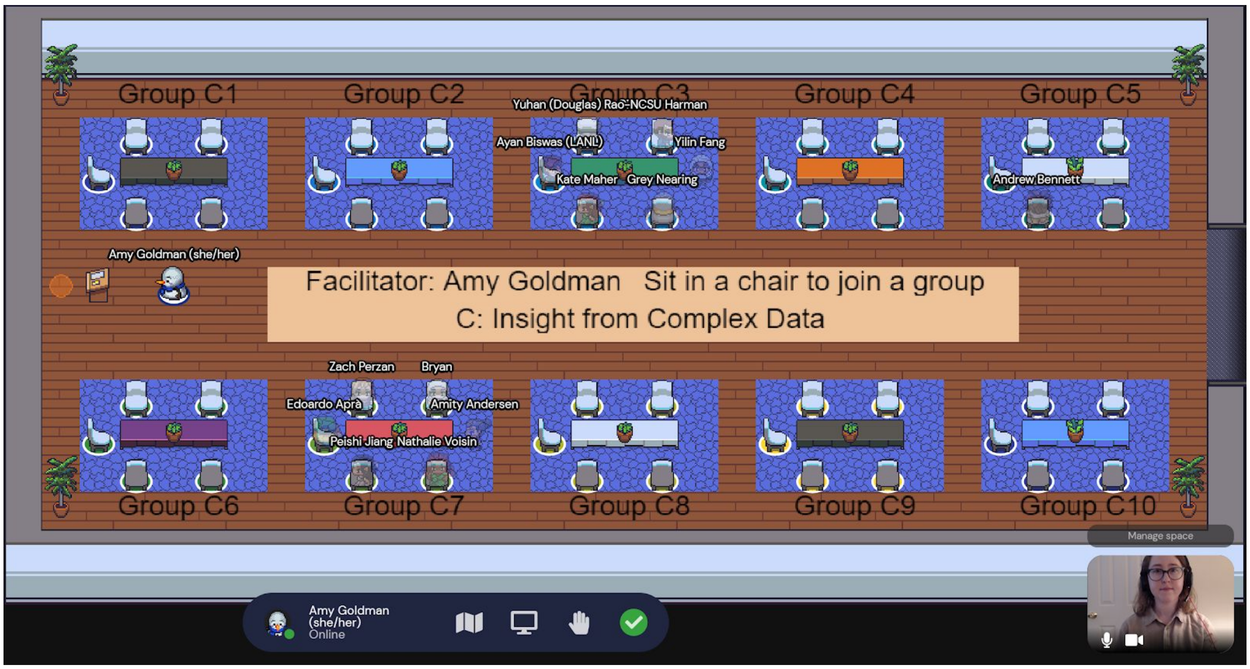

Figure 1. One of three topic-based rooms in Gather.Town: Topic C - Insight from Complex Data. Attendees moved their avatar into a chair around a table and then interacted with the other attendees at the same table for subsequent activities. A facilitator led the groups through the activities based on the "S^3" approach.

Within these breakout groups, attendees used Google JamBoards to write solo ideation post-it notes, and subsequently shared them with their small group (i.e., within their table). These post-its notes were synthesized by each team to fall within three to four themes. Each breakout table then used Google Docs to expand one theme into a white paper concept using a provided template. After completing the templates, attendees moved from Gather.Town back to MS Teams, where each group/table shared their white paper concept to all workshop attendees via a three-minute flash talk. Each white paper concept had a pre-populated link to join a separate MS Teams meeting dedicated to further developing each white paper. Regardless of which group an attendee was part of they were free to join any white paper team. After a period of further development within each white paper team, all attendees came back together to share outcomes and plans for a final time. After that sharing session, the facilitated portion of the ideation session was complete. Each team was then on their own to pursue their white paper as they deemed appropriate.

Outcomes. The ideation had 122 registered participants from 36 institutions spanning national labs and academia. The number of individual ideas generated are too numerous to count and were rolled into numerous white paper teams (up to 14) distributed across all three focal theme areas. The long-term influence of these white papers is impossible to predict or quantify. Given that the session achieved a significant amount of diverse idea sharing and synthesis (across institutions and disciplines) that would not have occurred otherwise, we strongly believe that the session has provided important concepts to help BER achieve its vision of dramatically improved Earth system predictability.

In addition to conceptual outcomes, we believe the vision, philosophy, and approach of the ideation session is paradigm shifting in terms of how we collectively interact, share, and work together towards scientific challenges bigger than any single person, team, or institution. Feedback was solicited via a survey at the end of the session, and participants also provided unsolicited feedback in real time. In both cases, the feedback was very positive, in particular about the dynamic integration of MS Teams, Gather.Town, and Google JamBoards. In addition, 100% of survey respondents said they would participate in a similarly structured virtual workshop; this is a remarkable outcome given 100+ participants in a virtual setting. Maybe most importantly, the idea session brought more researchers and their ideas to bear on BER's AI4ESP challenge that would have participated otherwise (Figure 2).

The ideation session had successes in terms of providing a platform for dynamic ideation, synthesis, and team building. However, the session also faced challenges. In particular, it took some time to get everyone familiar with Gather.Town as an application that most had not used previously. There are also some limits to functionality of Gather.Town. For example, some participants had trouble contacting their room facilitator when help was needed. There are simple solutions to many (not all) of the technical challenges that only require more upfront guidance. In addition, Gather.Town is free only up to 25 participants and beyond that is $3 per participant per day. Despite the challenges, the platforms worked well together and a goal going forward is to build more familiarity with all the platforms, develop new ways to dynamically integrate them, and address technical pitfalls with more formalized guidance.

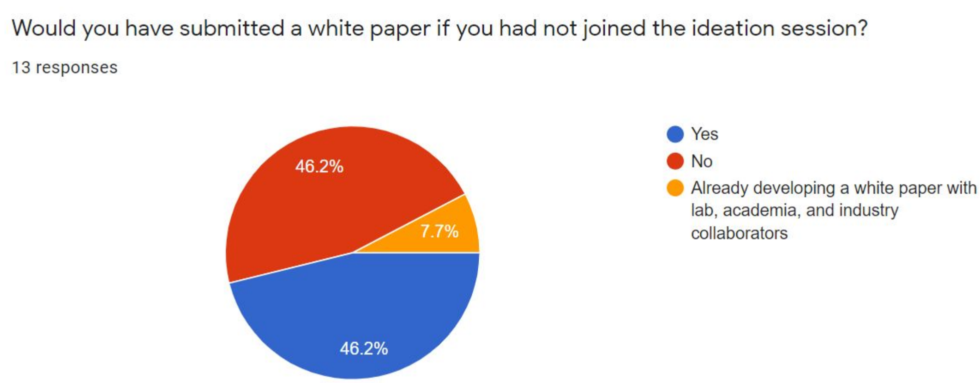

Figure 2. The post-session survey found that nearly half of respondents would not have contributed to a white paper without the ideation session. While only 13 participants responded, if we assume this is a representative sample, the ideation session may have brought many 10s of additional researchers and their ideas to bear on BER's AI4ESP challenge. Other survey outcomes indicated strong support for the session's novel approach to large-scale virtual ideation and synthesis.

Section 2: An Emergent 'Meta Idea' Spanning all Focal Area Themes

<u>Motivation and Goal.</u> During the sharing of white paper concepts it became clear there were important opportunities to couple ideas within and across the focal theme areas into 'meta ideas.' The concept of a meta idea is one that is more than the sum of the parts, achieved

through mutual integration. All participants were invited to join the development of meta ideas, as outcomes of the collective effort. Our goal below is to provide an example of a meta idea spanning the three focal areas that goes beyond what any one focal area may achieve on its own. It is considered a community outcome led by Maruti Mudunuru.

AI-enabled ModEx to Better Understand and Predict Extreme Events

Key question. Traditional machine learning (ML) methods require high-quality and massive datasets to make reliable predictions. Typically, data on extremes are sparse, uncertain, limited, and low-quality (e.g., having gaps and low signal-to-noise ratios). When traditional ML methods are applied to these data to understand Earth system response under extreme events, they perform poorly. ***The scientific challenge we envision is how can we accelerate understanding of extreme events and prediction of their occurrence and impacts?*** Recent advances in physics-informed AI show promise to overcome this challenge. AI guided by physics holds the key to revolutionize the way we collect, analyze, and assimilate data into Earth system models. ***A key question to address is, "How can physics-informed AI dynamically guide the real-time collection and integration of high-quality data to better understand and predict extreme events?"***

Our vision. AI-based models developed in Focus Areas 2 and 3 ideation will help us to design better data acquisition systems. Specifically, physics-guided AI methods in Focus Area 2 provide fast, robust, and predictive emulators for automated data evaluation. Explainable AI techniques in Focus Area 3 ensure interpretability, thereby providing actionable insights (e.g., the value of information) from the acquired complex data. The combined efforts of Focus Areas 2 and 3 will provide us with a suite of AI-models to dynamically guide data collection. The efforts discussed in the ideation session also provided necessary methods to glean the high-throughput data towards identifying real-time patterns and signal of value to stakeholders (e.g., experimentalists, field-campaign personnel) to dynamically modify data acquisition strategies and overcome limitations.

Premise. **Why the need for better data acquisition systems?** State-of-the-art approaches for collecting representative data in Earth systems seldom capture water cycle extremes (e.g., impact of weather, drought, wildfires). This is compounded by ongoing difficulty in predicting these conditions. As a result, our ability to quickly and reliably assess Earth system responses (e.g., nutrient dynamics under extremes) is reduced considerably. Additional considerations need to be taken into account if these rare observations are of reduced quality, as this will introduce detrimental effects on the downstream pipelines (e.g., process models, making inferences and predictions). From a modeling perspective, the process model parameters representing extremes are unreliable, leading to poorly calibrated simulators and ill-informed interpretations. Within an economic framework, the amount of time, cost, and energy invested in collecting data representing extremes could be reduced. Physics-informed AI methods (e.g., through deep reinforcement learning) could be employed to inform data acquisition approaches wherein models inform the user how to strategically and dynamically modify acquisition strategies to maximize the usable information content of generated data.

Research gaps and proposed approaches that use AI-models built on Focus Area-2 and Focus Area-3. Currently, most of the AI research focuses on inventing new algorithms that drive better predictions. However, these algorithms are data-driven. They require massive amounts of high-quality data for improving predictions on extremes (e.g., the evolution of hydro-biogeochemistry after drought, wildfire). Unfortunately, capturing these climate water cycle extremes and associated processes using current observations is intrinsically limited. This is because the opportunities to sample extreme events are rare. Also, there are several practical (e.g., mechanical, system-level) limitations of climate user facilities (e.g., DOE ARM) when documenting extreme event behaviors. As a result, current AI-models are not equipped to better predict ecosystem response to extreme events. To overcome this limitation, we rely on the AI-models developed in Focus Area-2 and 3 to develop an active learning-based feedback loop. For example, physics-guided deep reinforcement learning can be used to develop such a loop. This AI-enabled active feedback results in better data acquisition approaches and physics-informed strategies to characterize the water cycle under extreme events.

<u>How can Focus Area-2 help us collect high-quality data?</u> AI models developed through Focus Area-2 are trained using both data (if available) and physics [e.g., 1,4-11] that can represent extremes (e.g., see Table-1, Ref. [1], which provide a suite of disturbance models). Physics-based ML methods such as neural ODEs, graph neural networks, physics-informed neural networks (PINNs) [6,10], physics-informed coKriging [11], approximate Bayesian methods [10], and other methods using a functional representation of unknown physics, parameters, and quantities of interest [4,5,7-9] are used to develop the AI models. Note that each functional representation of extremes introduces bias. An approach to overcome this problem is to use recent advances in unsupervised learning (e.g., autoencoders, matrix/tensor factorizations). A primary goal of the associated AI is to identify extreme event patterns. This is achieved by differentiating between (1) noise, (2) normal process, (3) possible extremes based on functional representations, and (4) extremes that are not expressed in functional representations. If collected data does not fall in (1), (2), or (3), it is an outlier. This automatically identifies whether we are collecting high-quality data that falls in the category (i.e., category 4) needed to dramatically advance our understanding and predictive capacity around impacts of extreme events. If we have category 4 data, we can update our functional representations to develop new physics associated with these data. Furthermore, this strategy will identify when and where category 4 data gaps exist, and the types of data that are needed. In turn, we envision real-time nimble deployment of the necessary measurement systems to fill the identified gaps. There are significant opportunities to achieve this kind of dynamic, real time deployment through an approach that coupled researcher-deployed instrumentation with highly distributed crowd sourcing of required data. The key is building data acquisition systems that are extremely scalable for nimble deployment into targeted points in space and time. Investment in this vision for data acquisition may be the primary bottleneck of our vision. Overcoming it with heavy use of proxies from existing data acquisition systems (e.g., remote sensing) will be paramount. Critically, physics-based ML methods can directly exploit conservation laws and are sample-efficient. As a result, they can identify extreme event patterns even under limited data (e.g., through unsupervised deep learning). To train these physics-informed AI-models, extensive data representing extremes is not needed as compared to data-driven models. This is vital to align model data needs with what is possible for data acquisition.

<u>How can Focus Area-3 help design better data acquisition systems?</u> Explainable AI-based models developed in Focus Area-3 glean complex data (e.g., from multiple sensors, heterogeneous data sources sampled at different frequencies, metadata) to verify the quality of collected data. Physics-informed generative adversarial networks [e.g., [2,3,9,12]] provide reassurance on data fidelity. For instance, a deep and more generalized understanding of data can be achieved through deep Taylor decomposition, SHapley Additive exPlanations (SHAP), and local interpretable model agnostic explanations [2,3]. Moreover, interpretability will result in context-aware AI-controlled systems, which leverage Observing System Simulation Experiments (OSSE's) and collected DOE datasets to control instrument (e.g., DOE ARM user facility) operations. The outcomes can be coupled with physics-informed AI outcomes (Focus Area-2) to further guide/refine in real-time the nimble, targeted data acquisition strategy summarized

above. As a result, we will have the capacity to predict extreme events, target data acquisition to the associated places, times, and most relevant data types. The goal is dramatic improvements to our ability to understand and predict the occurence and Earth system impacts of water cycle extreme events.

Expected outcomes. The resulting integrated system of AI-models coupled to nimble, targeted data acquisition will inherently feedback upon itself leading to continuous improvements in predictive capacity, knowledge, and optimized data generation. That is, the system will automatically and continuously identify and execute field-campaigns needed to better sample, understand, and predict extremes. This includes spatio-temporal locations of samples/sites and critical data types and processes from sources such as remote sensing (e.g., using ARM), pre-existing models (e.g., E3SM, ATS, PFLOTRAN, E4D), FAIR data repositories (e.g., ESS-DIVE, WHONDRS), and new physical samples or crowd-sourced 'on the ground' real-time data. Without such a system focused on extreme events, the research community will continue to chase these events without the coherent, integrated model- and data-driven structure needed for paradigm-shifting advances in predicting how the Earth system responds to water cycle extremes.

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