Federal Register Notice 86 FR 46278, https://www.federalregister.gov/documents/2021/08/18/2021-17737/request-for-information-rfi-on-an-implementation-plan-for-a-national-artificial-intelligence, October 1, 2021.

Request for Information (RFI) on an Implementation Plan for a National Artificial Intelligence Research Resource: Responses

National Energy Technology Laboratory

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In 2020, The U.S. Department of Energy's (DOE) Office of Fossil Energy & Carbon Management (FECM) and the National Energy Technology Laboratory worked with other DOE applied energy stakeholders to evaluate and constrain Artificial Intelligence (AI) research and development (R&D) resource needs for our Applied Energy R&D Office. These findings were used to produce the report that follows, which aligned to the Office of Science and Technology Policy's (OSTP) and the National Science Foundation's (NSF) ''Request for Information (RFI) on an Implementation Plan for a National Artificial Intelligence Research Resource.'' While developed for addressing the AI/ML needs of FECM, the recommendations in the report may address the needs of AI/ML researchers in other areas to support and produce more efficient and effective products and breakthroughs.

Accelerating FECM R&D Using AI and ML

The U.S. Department of Energy's Office of Fossil Energy & Carbon Management (FECM) supported researchers are now applying artificial intelligence (AI) in at least 70 applied research and development (R&D) projects.[1] Most of these projects remain in early development, and all focus on solving known challenges within specific program areas. To evaluate FECM's readiness to better leverage the full power of AI, an internal AI Guidance Team was formed to examine existing gaps in AI capabilities and untapped opportunities for AI to broadly accelerate FECM research.

As a first step, the team reviewed the exceptional AI/ML resources and unique capabilities being developed at FECM's National Energy Technology Laboratory (NETL). Next, the team focused on the hurdles that currently impede or restrict FECM's use of this transformational technology. This paper summarizes the team's findings and recommendations.

Findings of the FECM AI Guidance Team

AI in FE: Hurdles & Recommendation

Data Hurdles. Researchers today spend too much time and effort to find, obtain, and prepare enough high-quality data with the properties and formats needed to drive targeted AI/ML solutions.

Tools Hurdles. It is also hard for researchers to find the right AI tools, so they often develop them from scratch. FE lacks a secure, central hub for developing, storing, and evaluating *models and algorithms*.

Computing Hurdles. Gaining access to the computing power required for AI/ML work can be challenging. Settling for suboptimal computing resources can waste enormous amounts of time, money, and energy.

Recommendation

FE should accelerate efforts to stand up a secure, integrated AI/ ML development environment that provides researchers seamless access to the tools, data, and resources required for rapid AI-enabled breakthroughs in the FE mission space.

[1] Note: AI is used broadly to include machine learning (ML) and other AI subareas.

FECM has no shortage of promising applications for AI, and access to an **integrated AI/ML development environment** could significantly accelerate the pace and broaden the scope overall. A foundational AI/ML development resource that provides vast libraries of curated data; proven, interoperable tools; expert AI support; and access to the necessary computing resources (see Figure 1) will significantly expedite FECM progress and reduce AI project costs.

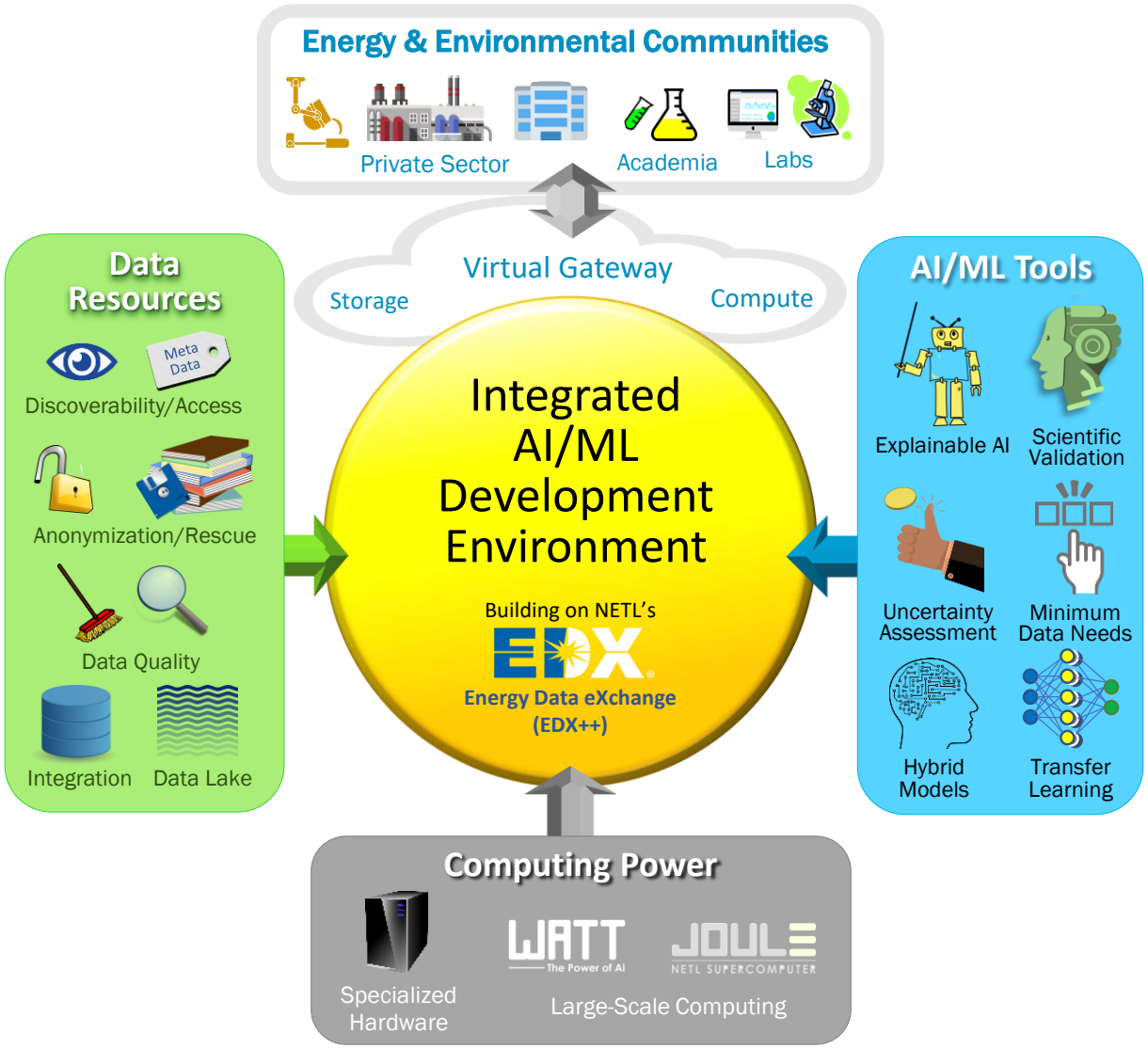

Figure 1. FECM seeks to build on NETL's powerful existing AI resources, particularly its **Energy Data Exchange** to integrate critical resources for AI into a central, curated system that provides diverse DOE research teams

FECM's AI Guidance Team recommends explicit R&D activities and other actions that FECM can pursue to accelerate larger AI benefits. These findings align with those of the recent Secretary of Energy Advisory Board (SEAB) *Final Report on AI/ML*, which calls for a *DOE-wide*, integrated AI capability, among other resources. A draft final report by the National Security Commission on Artificial Intelligence[2]

[2] National Security Commission on AI, Jan. 2021: www.nscai.gov/wp-content/uploads/2021/01/NSCAI-Draft-Final-Report-1.19.21.pdf

similarly stresses the need for such a resource at the national level. The proposed integrated AI/ML resource at NETL could expand over time to help support a progressively larger (DOE-wide) AI/ML development environment.

Building an integrated AI/ML development environment will provide current and future FECM researchers ready access to vast, curated data sets; state-of-the-art AI tools; specialized computational resources; and a safe, collaborative environment (fully compliant with all applicable cybersecurity protocols and practices) in which to develop, test, and optimize products or solutions. Recommended R&D to create this resource is outlined below in each of the three categories shown in Figure 1.

The FECM team's R&D recommendations on AI are closely linked and often interdependent. These dependencies indicate that implementing only a narrow subset of these recommendations, rather than the entire suite, could significantly degrade overall benefits.

Challenges: Although FECM holds an enormous volume of project data that could now drive transformative AI/ML solutions, FECM researchers today find it hard to know what data exists, where it is, what format it is in, who owns it, and other critical characteristics. Robust data curation and management tools could facilitate AI breakthroughs in plant operations and maintenance; carbon capture and storage; resource prediction, extraction, and protection; and energy storage.

Data Resources

FECM/NETL has amassed extensive (billions of attributes and features, PB of datasets), unique data sets in diverse formats and storage media (including journals, mainframe tapes, and floppy discs)—and continues to generate massive amounts of new data every day. Industry, university partners, and others also hold vast quantities of raw and sometimes proprietary data that FECM could use AI to transform into a useful knowledgebase for its stakeholders.

Data analysts now often spend up to 80% of their time just locating, obtaining access to, evaluating, formatting, and/or otherwise preparing the right data for each project.[3] FECM's AI Guidance Team identified the following R&D activities to potentially flip this paradigm—so that analysts and researchers can readily identify and prepare all relevant data—accelerating research progress and ultimately yielding better outcomes.

Recommended Actions: Data Resources

Caveat: In carrying out the recommended actions below, it is imperative to actively protect and preserve all existing workflows and data sharing agreements with industry partners. Access to these essential, high-value data sets relies heavily on our partners' trust in DOE confidentiality—a trust that must be upheld.

"One of the major scientific challenges of our time is being able to access and effectively analyze mounting quantities of data."

Dr. Chris Fall, Director, DOE Office of Science

[3] Crowdflower, 2016: https://visit.figure-eight.com/rs/416-ZBE-142/images/CrowdFlower_DataScienceReport_2016.pdf

Discoverability/Access — All new and existing data sets should include accurate meta data to summarize basic information about the data (e.g., type, dates, ownership, format, etc.). Meta data is a feature of the widely embraced **FAIR** principles to improve the **F**indability, **A**ccessibility, **I**nteroperability, and **R**euse of digital assets.[4] To the extent practical, FECM can increase data discoverability by fostering broad adoption of FAIR principles and best practices across FECM-funded research. An early step in this direction is to develop boilerplate language for future **Funding Opportunity Announcements** (FOAs), specifying partner adherence to FAIR principles. Care should be taken to avoid unduly burdening primary investigators and to protect proprietary data if the owners are not satisfied with anonymization techniques (as described below).

Once FECM has marshalled its unique and valuable data sets, the resulting searchable, curated collection will significantly improve data discoverability. This resource can raise the participation level of potential data contributors, demonstrate tool proficiency in preparing data for specific applications, and streamline storage requirements.

Data Anonymization and Rescue — AI tools tend to improve with more data, so the ability to share data across widening scales (materials, devices, plant, company, industry) should produce more robust models that can make better predictions and decisions. Steps to increase data sharing include data anonymization tools and the rescue of legacy data. At present, many utilities, power plants, industries, and other businesses may resist sharing their raw data, fearing risks to security and customer privacy. **Data anonymization tools** can prevent data from being traced to its source, but the tools currently available offer a range of security levels, and the best require significant time and investment. FECM R&D could improve the security and cost effectiveness of anonymization tools to make owners of proprietary data more willing to share their data and help generate AI tools that optimize operations across industry. Similarly, FECM needs to mount a major effort to find and develop **meta data for all existing and legacy data sets**—including those stored on mainframe tapes, paper files, floppies, and other hard-to-search formats. DOE invested in the collection and retention of this data, and it could potentially help drive future AI solutions. FECM must also plan now to avoid *future* legacy issues.

> "Although DOE has access to vast amounts of data and can potentially collaborate with industry to gather additional data, the quality and format of data and protecting the data are issues that need to be overcome."
>
> SEAB AI/ML Final Report , p. 56

Data Quality — Researchers need to thoroughly understand the quality of their data—including its lineage, robustness, and uncertainty. These properties vary widely by data set, and quality requirements vary by application. FECM needs a range of methods and tools to determine data quality, assess accuracy, and detect flaws. Tools are also needed to rank, cleanse, reconcile, and upgrade the data. AI-based tools could potentially make this process fast and inexpensive.

[4] GO FAIR, FAIR Principles: www.go-fair.org/fair-principles/ See also DOE awards $8.5M for FAIR data to advance for AI, August 10,2020.

Data Integration — FECM needs reliable tools and protocols for managing and integrating data assets in diverse formats and from diverse sources (other federal agencies; state, local, and tribal governments; commercial enterprises, etc.). Broad use of consistent standards would significantly expand options to create rich, application-tailored data sets. However, multiple standards exist within sectors, and convergence on a common standard will take time to emerge. FECM is well-positioned to conduct research and development efforts to create software-based tools with the following functionality:

- Parse through data for consistency
- Combine multi-source, multi-format data
- Convert data to compatible formats
- Extract or compress massive scientific data sets
- Automatically upgrade/update data from the source
- Create archives to prevent loss of investment in data
- Validate models and simulation tools

Data Lake — FECM should work with its partners and data sources on the best parameters and protocols to set up a secure "data lake" containing indexes to a diverse range of data sets. FECM needs a secure data lake to facilitate raw data discoverability and access with the ability to query data owners. The unstructured data potentially provides users great flexibility and value.

AI/ML Tools

Researchers who use traditional models based on mathematics and physics typically have little difficulty in following the logic of a model. In contrast, AI models and algorithms derived from patterns identified within large volumes of data are not amenable to human interpretation. The task is intensified in deep neural networks, which autonomously learn domain features by imprinting patterns on multiple interconnected layers of simulated artificial neurons (nodes).

While AI has a proven ability to turn massive amounts of data into useful insights, the technology continues to be a "black box," which raises legitimate concerns: Is the model biased because it was trained on inaccurate or skewed data? Is it making decisions based on faulty patterns or relationships (e.g., traceable to a sensor error)? Users need to feel completely confident in AI models to harness their potential for problem solving and system optimization.

Challenges: AI models are inherently complex, driving the need to understand and validate model outcomes. Tools and protocols are needed to identify or mitigate bias, eliminate faulty logic, and test accuracy, often with the use of improved data. Such tools are essential to lower the risk and boost acceptance of AI.

Finding the most relevant AI models for a specific project can also require an inordinate amount of time, particularly if models are isolated in diverse silos within programs or application areas. Researchers need the ability to quickly locate a model and discern its functions, optimal uses, and data requirements.

Recommended Actions: AI/ML Tools

Explainable AI — FECM needs reliable tools to explain what its AI algorithms and models are doing. The goal of 'explainable AI (XAI)' is to explicitly show a model's strengths and weaknesses, steps in analysis, and the factors that most influence the outcome (see Figure 2). Emerging XAI models often incorporate an interface that offers data visualization (to explain relationships among specific data features) and scenario analysis (to show how various input values affect output). Key advantages of XAI are improved debugging, faster adoption, and improved ability to audit ethics adherence.[5]

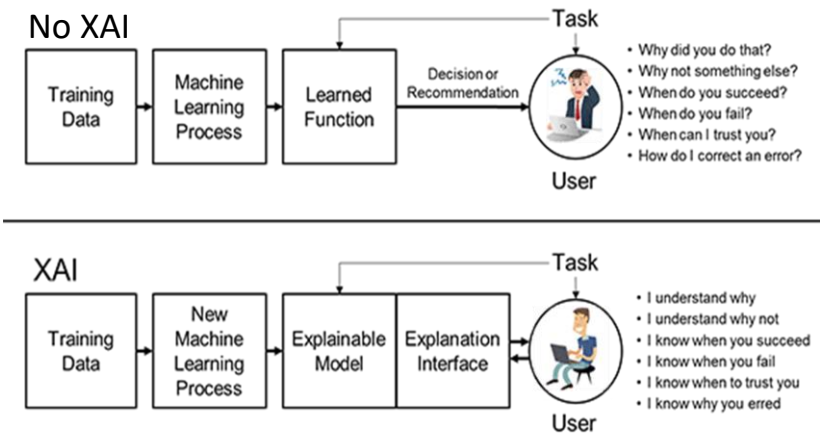

Figure 2. Explainable AI helps clarify how an AI model operates. DARPA

Scientific Validation — Given the science-based nature of FECM R&D, the new patterns or relationships exposed by AI must be validated by subject matter experts in the relevant disciplines. Domain experts must collaborate with AI specialists to help make sure that each model follows the science and does not violate any physical laws (e.g., the second law of thermodynamics).

Uncertainty Assessment — Users of AI models need to understand the amount of uncertainty in each model's conclusions or other outputs. Tools that quantify model uncertainty can guide efforts to improve the model and inform the appropriate level of trust in its predictions. FECM needs to invest in an integrated tool to help industry and other partners quantify the uncertainty of a model or algorithm for a given application (similar to CCSI).

Minimum Data Needs — FECM R&D has always collected and used massive amounts of data in support of scientific accuracy. In the subsurface, for example, the tenet that the confluence of disparate geographic and geologic factors make each site unique has stimulated intensive data collection, processing, and storage; however, all of the collected data may not be significant or even useful. Research to identify the truly critical data elements could potentially save vast amounts of time, money, and effort. To the extent research can identify the critical data elements, tools would also be needed to select and more efficiently store only the useful pieces of data.

[5] AI Multiple, Explainable AI (XAI) in 2021: Guide to enterprise-ready AI, January 1, 2021. https://research.aimultiple.com/xai/

Hybrid Models — As AI evolves, opportunities exist to leverage and expand model capabilities. FECM can explore the benefits of combining and augmenting models. For example, pre-trained neural nets might be combined with science-based models; to achieve this, a neural net might be trained using empirical data as well as data from a physics-based computational model.

> "Those charged with utilizing AI need an informed understanding of risks, opportunities, and tradeoffs. They need awareness of the possibilities and limitations in a system's expected performance."
>
> *National Security Commission on Artificial Intelligence, Final Report*

Transfer Learning — The initial training of a neural network typically requires intensive use of data, time, and computing power. Once trained, neural networks often require minimal additional training to become useful in applications that are similar to—yet distinct from—the one for which they were originally created. This ability to transfer the learning from an existing neural network can significantly expedite AI results and lower costs for new applications. Curated tools may be developed to help identify previously trained neural networks that are potentially relevant to an application.

Computing Power

Challenges: AI-associated computing creates the need for improved access to high-performance hardware, greater speed, and optimized computer architectures. Associated concerns include cost and power usage.

Even as advances in AI yield impressive results, concern is growing over the availability, power consumption, accessibility, and cost of today's supercomputers, which are used to train deep neural networks. The rapid growth in AI computing requirements raises questions about access to high performance computing (HPC) capacity. Efforts to expand AI must consider equity and other impacts. FECM maintains top-tier computer resources at NETL and recently created the *HPC for Energy Innovation Initiative* to give industry and other partners the computer access they need to explore new energy technologies. Additional solutions involve the use of cloud computing, scaled models for edge computing, more energy-efficient algorithms, tools for tracking the carbon footprints of algorithms, and more efficient chip architectures. An integrated AI development environment must provide seamless access to adequate and appropriate computing power.

Recommended Actions: Computing Power

Large-Scale Computing — FECM enjoys access to two (2) large-scale computers through NETL: **JOULE** and **WATT**. The Joule 2.0 supercomputer lets researchers simulate challenging phenomena and run high-fidelity modeling tools at various scales (molecules to entire plants or carbon storage formations). A talented mathematician working 40-hour weeks for 50 weeks per year would take about 55.9 billion years to do what Joule 2.0 can do in one second.[6] The WATT computer provides large data storage and analysis capabilities that use cutting-edge algorithms

[6] NETL, Using Artificial Intelligence in Fossil Energy R&D, April 9, 2020: www.energy.gov/fe/articles/using-artificial-intelligence-fossil-energy-rd

and harness the power of AI and ML to address previously unanswerable problems. To maintain the value of these computing resources and keep pace with evolving requirements, FECM/NETL must continuously refresh and update these systems, integrating the latest architectures and increasing capacity.

Specialized Hardware — FECM can immediately and dramatically increase the speed and efficiency of its neural net training by acquiring new, specialized hardware. As an example, Cerebras' powerful and compact new hardware is designed specifically to train complex neural networks. Cerebras' giant chip performs this task considerably faster than large, general-purpose computers like JOULE. It also takes less space and uses far less electricity. The unique architecture of this AI hardware will provide NETL the opportunity to develop specialized software, which translates into the following:

- Faster and cheaper development of AI/ML models for real-time control and optimization of carbon capture systems, industrial plants, and power plants, improving fuel flexibility, reliability, and emissions reduction.
- Rapid development of physics-based models used for computational fluid dynamics or for the optimization or troubleshooting of power plant devices and industrial systems.

Integrated AI/ML Development Environment

Efficiently implementing the R&D activities described above and incorporating the results into NETL's existing Energy Data Exchange (EDX) network will give FECM the expanded development environment it needs to vastly accelerate AI/ML solutions *across its mission space*. As envisioned, this integrated environment will provide authorized AI researchers rapid data discoverability and streamlined access to robust data sets; tools and models; custom, secure workspaces or sandboxes; computing power; and cloud-based resources—all in compliance with federal cybersecurity requirements.

NETL is a natural choice to host this integrated AI/ML development environment. The Lab is an active participant in cooperative AI research activities across the National Laboratory System (NLS), provides specialized curation and access to large scientific data sets through EDX, serves as the lead DOE facility for geo-spatial data; and cooperatively shares its AI expertise, data tools, and computer resources among diverse FECM/NLS research communities. As a government-owned, government-operated (GOGO) lab, NETL is well positioned to serve as a user facility for all of FECM (with potential for future expansion), expediting progress on AI/ML-assisted research. The proposed development environment will be designed to:

- Preserve current interfaces for distinct FECM research communities and programs
- Facilitate access to the necessary data, software, and computing power
- Ensure automatic compliance with all applicable federal cybersecurity requirements
- Provide tailored sandboxes and expert IT support
- Reduce duplication of effort and streamline routine activities.

As host of the proposed AI/ML environment, NETL will continue to work with its sister labs and strengthen NLS foundations for advanced AI, physics-informed ML, deep learning, and neural

networks. The following important FECM/NETL/National Laboratory programs are a few of the many research communities that can leverage this integrated environment to accelerate progress in key areas:

- **Materials discovery** (e.g., eXtreme MAT)**.** Improving the efficiency and economics of materials for extreme environments/energy applications, such as:
  – Clean hydrogen production
  – Direct air capture
  – Advanced energy storage
  – Critical minerals
- **System optimization** (e.g., Institute for the Design of Advanced Energy Systems)**.** Supporting carbon-neutral systems in power plants and industry.
- **Offshore risk reduction** (e.g., Offshore Risk Modeling and related tools). Providing award winning data, tools, and science-based techniques to evaluate risks and security gaps in offshore hydrocarbon systems, including metocean and geohazards, analyze aging infrastructure to support the nation's offshore spill prevention environmental and social justice goals.
- **Subsurface prediction** (e.g., National Risk Assessment Partnership and **S**cience-Informed **M**achine Learning To **A**ccelerate **R**eal-**T**ime Decisions). Reducing risks and improving the efficiency and environmental sustainability of subsurface exploration and carbon storage.
- **Carbon capture technology** (e.g., Carbon Capture Simulation for Industry Impact). Providing a virtual learning environment to accelerate the deployment of complex engineered systems in power and industrial applications

Recommended Actions: Integrated Development Environment

Integrated AI/ML Development Environment — As currently conceived, a qualified user could gain access to all the resources in FECM's Integrated AI/ML Development Environment from their preferred development environment, such as IDAES or MFIX, via an application programming interface (API). Once connected, users will be able to:

- Search indexes in the data lake to find data sets of potential interest and pull them into the workspace, observing applicable owner requirements (if any).
- Search for algorithms, models, trained neural networks, or other software suitable to the application and pull them into their workspace.
- Schedule time on computing resources to run the software.

The sought-after data sets, models and tools, and computing resources may physically reside at NETL, within the NLS, on a Git site, on the cloud, or elsewhere.

As envisioned, approved users will eventually also have seamless access to anonymized raw data made available by external partners, including industry (following a formal permission process). In exchange for the data, these organizations may access continuously improved

algorithms or models suitable for in-plant or on-site use to optimize operations and efficiency (edge computing).

Virtual Gateway — NETL will develop a virtual gateway to the integrated AI/ML development environment to streamline entry while meeting all federal cybersecurity conditions and protocols. Building on the current portal to the EDX database, NETL will streamline tiered access by researchers who previously passed requisite cybersecurity checks and received approval. The resources to which they have access will be controlled automatically in accordance with clearance and project need.

Staff Expertise — NETL must have a highly qualified team to handle growing system capabilities and rapidly evolving cyber threats. Launching and maintaining a safe, efficient, and secure integrated AI/ML development environment will require close coordination among a team of experts in three areas of specialization:

- **Systems Administration.** To effectively manage the configuration, upkeep, and reliable operation of the integrated, multi-user computer system.
- **Cloud Systems**. To manage integration of increasingly complex cloud services with existing data, software, computing, security, and research requirements.
- **Research Science and Cybersecurity**. To maintain full compliance with federal cybersecurity rules and assure ongoing protection of hardware, software, and data systems from cyber threats while preserving required functionality for research.

Git Account — Setting up an enterprise-level account on a Git hosting service will give FECM researchers and other authorized users access to tools on other Git sites and allow them to catalog and store specialized models and other software on a single, easily accessible site. To store a new or improved software tool, users may apply to upload it to the Git. Once approved and posted, all users could gain access to these tools.

Summary

The recommendations outlined in this paper are designed to address gaps and supply the components needed so that FECM can rapidly harness the full power of AI to solve the pressing challenges now facing the energy sector and the nation. AI's potential to optimize systems and predict events or outcomes can expedite DOE progress toward net-zero carbon emission, social and environmental justice goals while supporting efficient innovation of next-generation energy technology and knowledge development.

The strategies and needs identified here for AI in FECM research programs are likely to complement those of other federally funded research programs. Therefore, the recommendations of this paper are provided for the RFI reviewer's consideration in support of their broader, national goals.