ANL-23/69

ADVANCED RESEARCH DIRECTIONS ON

AI FOR ENERGY

Report on Winter 2023 Workshops

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U.S. DEPARTMENT OF ENERGY

U.S. DEPARTMENT OF ENERGY | Office of Science

NNSA National Nuclear Security Administration

April 2024

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Advanced Research Directions on AI for Energy

Report on the U.S. Department of Energy (DOE) Winter 2023 Workshop Series on Artificial Intelligence (AI) for Energy

Program Committee

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Special Thanks

To the Argonne National Laboratory Communications and Public Affairs Division's Writing Center of Excellence, including key support from Andrea Manning and Lorenza Salinas

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EXECUTIVE SUMMARY

Artificial intelligence (AI) provides a transformational opportunity to rapidly deploy new clean energy, secure critical grid energy assets from threat actors, and reduce capital and operational costs of next-generation energy technologies and the connected systems that embody the demand side of the transformation. The United States will need to invest trillions of dollars in energy infrastructure to reach the nation's clean, resilient goals by 2050. At the Department of Energy (DOE) national laboratories, AI has incredible potential across nuclear, renewable, and carbon management domains due to the ability to represent unprecedented system model sizes, provide intense computational resources, and capture knowledge from a workforce of the nation's top scientists. In aggregate, AI could reduce the cost to design, license, deploy, operate, and maintain energy infrastructure by hundreds of billions of dollars if the following applied energy challenges are realized.

EXEMPLAR GRAND CHALLENGES FROM THE CHAPTERS OF THE AI FOR ENERGY REPORT

01 Nuclear Energy: Accelerating the Licensing and Regulatory Process

02 Power Grid: Building Cyber- and All-Hazards Resilient and Secure Energy Systems

03 Carbon Management: Realizing A Virtual Subsurface Earth Model

04 Energy Storage: Equitable and Accessible Deployment

05 Energy Materials: Advancing Beyond Material Properties and Performance to Achieve Lifecycle-Aware Materials Design

AI provides a breakthrough opportunity to accelerate the design, deployment, and licensing of new energy capacity. Commercial powerplant design and licensing are a multi-year effort that can account for up to 50% of time to market for new energy deployments. DOE estimates the onboarding of 1.6 TW of new solar capacity and 200 GW of new nuclear capacity, while enabling hydrogen, geothermal, critical minerals, and other clean energy resources by 2050, with a cost that could approach trillions of dollars in national investment to meet growing global clean energy demand. Additionally, DOE estimates the need to reduce costs to less than $100/net metric ton of CO_2 equivalent for both carbon capture and storage to address carbon pollution. AI has the potential to reduce schedules by approximately 20% across new clean energy designs, with potential savings in the hundreds of billions of dollars by 2050. Additionally, AI can augment and extend the energy development workforce that will be in high demand.

The energy grid's generation capabilities and demand-side needs are experiencing rapid changes in requirements for secure, reliable, and resilient planning and operations controls. The increasing volumes of communications, controls, data, and information are growing the digital landscape, increasing flexibility and improving the reliability and agility of the grid by increasing visibility to operators and consumers. Integrating energy systems together across grid operations could save billions of dollars annually by automatically optimizing generation and demand-side needs.

Autonomous operation technologies can provide monitoring, control, and maintenance automation across various clean energy technologies. Distributed, consumer-sited technologies are changing the power load with electric vehicles (EVs), distributed storage, smart buildings, and appliances adding new intelligence to loads while also requiring the integration of consumer-sited controllability. Furthermore, new advanced nuclear technologies, such as microreactors, will likely need to operate autonomously to realize economies of scale. Delivering AI capabilities across the operations and maintenance lifecycle can transform safety, efficiency, and innovation within national energy production and distribution infrastructure.

The siting of new energy capacity is a complex challenge balancing energy generation options, community needs, environmental factors, and resiliency considerations. AI could aid community energy planning based on a comprehensive dataset and a trained community energy foundation model that captures characteristics of and interactions between physical infrastructure, human behavior, and climate/weather impacts. AI tools can achieve national clean energy goals by democratizing community-level clean energy resources and facilitating the identification of energy transition pathways that reflect local objectives, demographics, and legacy infrastructure.

Natural disasters and human-caused events are occurring more frequently and with more intensity, delivering significant impacts to the nation. Adverse weather events are increasingly disrupting supply chains, damaging property and assets, and making certain areas less habitable. The U.S. experienced a record 28 unique weather/climate disasters that cost at least $1 billion in 2023. Climate change, urbanization, population growth, aging infrastructure, and deferred maintenance increase risks to communities and human survival. An AI-based, all-hazards global response system that has ingested global and stakeholder datasets, facilitating international preparation, response, and recovery, can enhance preparedness and resilience solutions and inform faster recovery.

Science-based models enhanced with AI multi-modeling approaches can improve predictions of subsurface properties and systems to improve resource discovery for domestic critical materials, geothermal reservoirs, uranium, and water opportunities. This capability could create a national subsurface AI and data testbed to enable responsible commercial, regulatory, and science-based discovery and development. AI can improve the forecasting and prediction of subsurface properties and systems, informing and transforming our ability to reduce risks and responsibly interact with the subsurface.

Energy material innovation is key to realizing national clean energy goals. Increasing automation in materials laboratories, such as autonomous laboratories, can transform the design and discovery of new materials. AI can also accelerate materials qualification through automation of materials testing, leading to new energy technologies such as advanced nuclear reactors and new battery certifications.

In addition to these cross-cutting opportunities, there are unique use cases in nuclear, renewable, and carbon management energy systems. For example, while emissions, prediction, measurement, and mitigation are uniquely important to carbon management, the underlying computational infrastructure could be shared across grand challenges. Unattended operation of nuclear reactors has unique life-safety considerations; however, many plant-level digital twins of piping, valve, heat exchanger, and cooling towers could be shared across applied energy domains. A DOE consortium model from all energy domains, integrated with expertise from subject-matter experts from the laboratories, could help ensure and drive efficiency across research challenges.

To accomplish these grand challenges, key developments are needed. The laboratories must establish a leadership computing ecosystem to train and host data and foundation models at ever-increasing scales. Fine-tuned models need to be developed for each domain that are coupled, where possible, with ground-truth, first-principles physics. Although the laboratories have hundreds of petabytes' worth of data, only small amounts of these data are cataloged, warehoused, and ready for AI model ingestion. Curation of one-of-a-kind, ground-truth data coupled with energy industry data will be essential to building models at these scales. Most important, partnerships across laboratories, government, industry, and academia are essential to realizing the transformational benefits of AI for energy.

This AI for Energy report further details grand challenges that provide significant opportunities for energy applications across nuclear energy, the power grid, carbon management, energy storage, and energy materials over the next decade. The main conclusions and opportunities from this study are available in the Key Findings section of this report.

INTRODUCTION

An important aspect of the U.S. Department of Energy's (DOE) mission is to ensure the nation's energy independence and security both in the short and long term. Key to meeting this challenge are continued advancements in artificial intelligence (AI), especially in the context of energy. As an initial step toward addressing these challenges, a group of about 100 experts on AI/machine learning (ML) and applied energy convened at Argonne National Laboratory in December 2023 over the course of two days to map out future needs related to utilizing AI. The goal of the meeting was to detail pressing technical challenges and propose AI-assisted solutions. Five domain areas were identified (detailed below), along with potential paths forward.

DOE is ideally positioned to address challenges associated with energy independence and security due to its unique set of assets. These assets include a highly skilled workforce with relevant domain expertise (nuclear engineering, chemistry, materials science, networked systems, etc.), and an array of world-leading experimental facilities for making advances in materials, chemistry, etc. These include synchrotron light sources, nanocenters, high-performance computing resources, and autonomous laboratories. By integrating these resources with other AI capabilities outlined in the previous AI for Science, Energy, and Security (AI4SES) report, the DOE can leverage AI to stay at the forefront of the rapidly evolving landscape. The applied energy focus described in this report centers on five areas vital to the energy future of the U.S., as well as underscores the critical role that AI can play in shaping our world—highlighting the urgency and importance of being leaders in AI to ensure impactful solutions to global energy needs. These areas include Nuclear Power, Power Grid, Carbon Management, Energy Storage, and Energy Materials. It will be essential to integrate these together and with other efforts in AI for science and technology. Complexity, the large-scale effort involved, real-time decision making required, robustness of systems, and safety implications all pose extra challenges. The grand challenges described in this report span multiple disciplines and have not been solved by conventional methods. The power of AI for solving such problems lies in its capacity to simultaneously handle multiple system characteristics while incorporating both data and specific domain (e.g., physics, chemistry, etc.) models and to do so on a scale and at a complexity otherwise not possible.

Nuclear energy plays a pivotal role in the clean energy landscape of the U.S., representing about half of its clean electricity generation. To achieve its full potential, the nuclear industry must adopt and, where required, advance the latest AI tools and technologies. AI's transformative potential is particularly relevant in methodologies which could drastically improve the economics of nuclear system design and operation. These challenges span multiple scientific and engineering disciplines and require AI's unique ability to process vast amounts of data and integrate physics models on a scale previously unattainable. This integration must be carried out in a seamless manner. AI can facilitate this coordination, potentially reducing costs significantly compared to traditional nuclear energy development and deployment approaches. Recent Generation III reactor commissionings have experienced notable delays and cost overruns, often due to premature construction starts. AI, developed under science and technology initiatives, can mitigate such issues by enhancing design completion and process efficiency. The intricate interdependencies within the nuclear energy sector pose challenges well-suited for AI solutions. While teams of experts might struggle with the breadth and depth of necessary knowledge — hampered by limitations such as succession planning and individual bias — AI offers unparalleled knowledge capture and the capability to discern cross-disciplinary connections. This advantage is critical in three specific challenge areas where AI/ML can surpass the performance of human teams: (1) streamlining the licensing and regulatory process; (2) accelerating deployment; and (3) facilitating unattended operation. Embracing and extending AI capabilities could significantly enhance the nuclear industry's efficiency and innovation, all while continuing to improve safety.

The global energy system, which powers the world's economy, is currently experiencing a transformation unparalleled since the introduction of electricity over a century ago. This evolution encompasses the shift toward a grid, characterized by enhanced computer control, communication, information exchange, and data analytics. Concurrently, there is a surge in smart, distributed technologies, exemplified by the widespread adoption of electric vehicles, photovoltaics, local energy storage solutions, and intelligent buildings and appliances. This transition is further complicated by increasing electrification and a significant shift in the primary energy mix toward more variable renewable energy sources, such as wind and solar power. The future management of the power grid introduces a level of uncertainty, particularly as parts of the grid come under diverse ownership and jurisdictional control, complicating future planning and operations. Recent developments in AI offer promising solutions to manage the future grid's intricacies. AI's potential to revolutionize energy system operations is vast, including by enabling proactive, real-time management; enhancing resilience and security against cyber and all other hazards; and facilitating the design and planning of a 100% clean electricity system by 2035.

In terms of carbon management, DOE's Office of Fossil Energy and Carbon Management (FECM) is dedicated to pioneering technologies aimed at reducing carbon emissions and lessening the environmental footprint of fossil fuel generation and usage. In pursuit of these goals, several grand challenges have been identified, including developing "disCO$_2$ver," a dynamic digital system designed for multi-scale simulation and forecasting to support interoffice and extramural collaborations. This test bed is crucial for speeding up the U.S. shift toward a carbon-neutral economy by improving greenhouse gas (GHG) mitigation and enhancing the resilience of energy infrastructure. Another significant initiative is the push to create a virtual subsurface digital twin, using AI to find, aggregate, and improve access to multi-modal data This endeavor will enable more environmentally friendly, clean energy resource extraction and secure waste and emissions storage. Additionally, efforts are focused on hastening the development and selection of optimal materials for large-scale carbon capture and removal. Where the transition to renewables will be more challenging (e.g., heavy industry), tools are needed for GHG emissions prediction, measurement, and mitigation. A future need highlighted is the ambition to render the earth "transparent" through AI and multi-modal data. The proposed solution encompasses utilizing a broad array of geophysical techniques to gather diverse data sets, employing AI to enhance sensor design and data collection, and leveraging AI for subsurface characterization.

Energy storage, independent of its source, whether renewable, nuclear, or carbon management, will continue to play a crucial role in future energy systems. The demand for improved (including much larger capacity) energy storage systems will necessitate diverse technologies to meet the varied requirements across different societal segments. The complexity and breadth of these requirements present a significant challenge in developing new solutions and doing so on the required accelerated time scale. As a result of the scale of the problem and the complex coordination required to develop and deploy these systems, traditional processes are too slow to respond to ambitious timelines. The challenges discussed in this document include accelerating the development of energy storage technologies; ensuring efficient deployment, operation, and control of energy storage systems; and guaranteeing that deployment is equitable and accessible to all.

Advances in materials science for energy applications are needed for generating, storing, and utilizing energy efficiently, encompassing storage materials, photovoltaics, thermoelectrics, catalysts, and advanced alloys. These materials are crucial for driving forward U.S. objectives in clean energy, economic growth, and energy justice, aiming to reduce reliance on nonrenewable resources and lessen environmental impacts. To meet the U.S. targets in sustainability and clean energy by 2050, there is an urgent need to hasten the discovery, design, production, and certification of energy materials with tailored properties and performance. This process involves navigating vast parameter spaces, far beyond manual exploration capabilities, and developing cost-effective, sustainable production methods while addressing durability and lifecycle management challenges. AI is significantly impacting energy materials research by accelerating material discovery and design, enhancing laboratory automation for quicker synthesis and testing, and facilitating the transition to industrial-scale application. AI's role is transformative, promising to lead to the discovery of new materials, predict their properties, and achieve breakthroughs to overcome energy sector challenges. Success in this domain could cement U.S. leadership in developing high-performance, safe, and environmentally friendly energy materials, supporting a shift toward a circular economy. The focus areas in this report include improving energy generation, storage, and conversion efficiency; enhancing environmental sustainability and scalability; and reducing energy production and use impacts. Addressing these needs requires new scientific and technological breakthroughs to accelerate material discovery, enhance predictive design, and bridge the gap from laboratory research to industrial application, moving beyond traditional trial-and-error methods for rapid material deployment.

In this report, the several recurring themes that have emerged include:

- The need for rapid and accurate in silico design and testing from materials, chemistry, and storage systems.
- The need for improved methods of quantifying uncertainties in predictions and system performance.
- The need for the use of AI to integrate multimodal data for both scientific and technological advances as well as for industry policy design, energy, and environmental justice.

KEY FINDINGS FOR ESTABLISHING THE CROSS-CUTTING ASPECTS OF AI SUPREMACY NEEDED TO ENSURE SUCCESS IN ENERGY MISSION AREAS

The energy mission areas — fossil, carbon management, nuclear, renewable, and energy efficient usage and delivery — have crosscutting needs for artificial intelligence (AI) technology. The nature of these needs is anchored in the high-consequence environment, the urgency, and the complexity of the systems involved. Establishing mission-ready technology in these areas builds a more robust and trustworthy capability that matures the baseline capability necessary to support exploratory research.

The five areas discussed during the AI for Energy workshop and consequent report cover large portions of the energy space and surface a robust set of capabilities that will also support the broader agenda. The primary conclusions include:

1. The potential for AI to have transformative impact on the energy mission critical to U.S. economic security is high.
2. It is critical for the energy communities to include research into AI technology development in order to cultivate the appropriate talent that can respond to crises that may emerge in the field and require interdisciplinary expertise to address.
3. The energy community needs are largely aligned with the six areas identified in the AI@DOE roundtable, as follows: energy efficient AI; intrinsically explainable AI; scientific generative AI; safe, secure, and trustworthy AI; AI for prevention, preparedness, and responding to national emergencies; and AI for automation.
4. Ensuring safe, secure, and trustworthy solutions has elevated importance in the energy mission areas, and rigorously assessing, documenting, and certifying AI technologies regarding these concerns are important differentiators from scientific discovery applications.
5. Investments in these general areas need to be pursued in an environment of use anchored in energy application areas to address the unique features of the energy area, and doing so will inherently increase the robustness of solutions applied in the science and security arenas. Such an environment can be created through a coordinated structure that combines the underlying crosscutting research with end-use applications.

In contrast to a traditional research environment, it will not be sufficient to employ a method that appears to work well — obtaining a good performance score on a battery of tests is not the endgame. The stakes are high enough in the energy space that we need methods that do not just work well but can be: (1) demonstrated to be provably correct, with known conditions of when they will break; (2) understood well enough to inspire confidence in the performance; and (3) supported by a workforce that can diagnose and correct problems. Solving this set of challenges ultimately supports security and discovery tasks, as well.

Success across the five energy spaces covered in this report will involve success in the areas of high-consequence, urgency, and complexity.

CROSSCUTTING ASPECTS NEEDED IN ENERGY MISSION AREAS

The following must be pursued across the five energy areas of nuclear energy, power grid, carbon management, energy storage, and energy materials

High-Consequence

- High-Consequence Decisions and Critical Operations
- Accreditation of AI Methods
- Trustworthiness and Verification and Validation (V&V)
- Development and Maintenance of Talent to Respond to AI Implications

Urgency

- Move at Speed of Field; Micro-Revolutions vs. Incrementalism
- Mission Imperative

Complexity

- Inverse Problems
- Robustness to Changing Environments
- Multimodal and Scalable

High-Consequence

HIGH-CONSEQUENCE DECISIONS AND CRITICAL OPERATIONS

- Planning, permitting, and design efforts span the energy areas and have implications for a decadal or longer timescale. The basis for decision support spans large amounts of legacy data (e.g., codes, standards, the existing built environment) that need to be aggregated with future resource and state estimates and policy drivers. These legacy data need decision coaches, that is, large language model (LLM)-like constructs that can handle natural language and scientific data. They would treat uncertainty and trade-offs as first-class constructs. They also don't hallucinate.

- Autonomous operations — of the grid, reactors, power plants, etc. — have no tolerance for failure. We need to reimagine control strategies based on methods that can provide guarantees. Core mathematics needs to catch up to heuristics for formalized design so that we encourage a different objective function, as in: "99% accurate 80% of the time, 50% accurate balance" is less desirable than "80% accurate 99% of the time."
- Low power solutions — for edge deployment (near instruments, field installations with limited connectivity, power-constrained applications).
- Scalable and distributed — grid operation and management of grid connected assets, as well as large fleets of deployed energy assets, have varying levels of connectivity and an intrinsic local versus global tension.

ACCREDITATION OF AI METHODS

- For practitioners to understand and document the performance of AI methods so that policymakers with a broader perspective can understand the implications of adoption of a particular method will require going beyond heuristics.
- Can we identify a scientific approach to AI methods development?

TRUSTWORTHINESS AND VERIFICATION AND VALIDATION (V&V)

- Robust methods for discovering vulnerabilities in a controlled and reproducible environment — such as deployment in DOE testbeds, white-hat adversarial AI, and standardized tests that benchmark performance — can leverage DOE's existing testbeds and facilities.
- Mathematics — formal methods, convergence guarantees —can be used to guide acquisition of expensive data. Imaging, sampling, and edge processing infrastructure are all very expensive in the energy world. Another question is: How much data is enough? This facet builds on DOE's commitment and track record of applying science expertise and understanding to chemical, biological, radiological, and nuclear (CBRN) threats, with technology specifically customized for the applied energy mission.
- Frameworks are needed for assessing data quality — in contrast to designed experiments, much of the data in the energy space is real-world observational. AI tools for assessing AI data, called cleaning, is a critical part of the chain in this area.

DEVELOPMENT AND MAINTENANCE OF TALENT TO RESPOND TO AI IMPLICATIONS

- We will need to maintain a talent pool involved in core research — the development of AI methods — with sufficient expertise to understand and correct vulnerabilities and shortcomings.

Urgency

MOVE AT SPEED OF FIELD; MICRO-REVOLUTIONS VS. INCREMENTALISM

AI research and development (R&D) tends to occur in microrevolutions; these are difficult for a workforce to track. In AI and ML, the methods tend to change rapidly. Many of the most popular approaches today didn't exist even a few short years ago. It would not be surprising if today's methods are overtaken by quite different ones in the very near future. The workshop explored how to conduct R&D and deploy the latest methods to energy applications in this rapidly changing environment – how to constantly retool the workforce. As the energy space needs solutions *now*: being a "slow fast follower" of the tech industry doesn't work. One challenge is how do we build the skillset that transcends the AI methods of the day and cultivate the expertise such that AI research advances innovation?

MISSION IMPERATIVE

- American jobs, economic security, and building the infrastructure to support high-quality way of life depend on safe secure and resilient energy supplies. Investment decisions are being made now that will persist for a generation. However, this pursuit of AI supremacy is not a long-term research project for energy — we need solutions now.
- Deployable AI technologies that leverage DOE's strong history of industry partnership are critical. The impact potential of AI for energy involves control of processes and infrastructure operated by private entities that may not have sufficient AI expertise to develop and correct problems with AI algorithms in the field. It is therefore necessary to accelerate the development-deployment-improvement cycle through AI algorithms that can be packaged for broad deployment outside of government. Such AI algorithms will minimize risk and self-identify improvement opportunities or possess self-healing capabilities, enabling close collaboration between DOE researchers and end users.
- Targeted discovery programs, such as catalyst development and alternatives to critical energy materials that relieve supply chain constraints for energy storage and

power electronics, can benefit from transformative productivity improvements with AI-guided material design and selection.

Complexity

INVERSE PROBLEMS

- Energy problems (e.g., subsurface sampling; storage device performance management; grid state; nuclear energy reactors) often allow for limited observations. Thus, there is a need to make decisions about the development of upstream and downstream infrastructure and deployment informed by information that requires solving inverse problems.

ROBUSTNESS TO CHANGING ENVIRONMENTS

- Truly autonomous operation — of grid resources, energy storage, and reactors — will inevitably put AI control algorithms in off-design conditions. The key features of prospective AI control systems are building in the ability to revert to "safe" behavior, calling for human intervention, and gathering the necessary data to enable rational decision-making.
- Methods that are robust to emergent behavior and incorporate robust uncertainty management to deal with situations where prior experience provides little guidance are needed.

MULTIMODAL AND SCALABLE

- The source data for energy problems is nearly always multimodal, such that the following must be brought together: time series, geographic information systems (GIS), network, natural language, and imaging; two-dimension (2D), 3D, and higher-dimension field data; and combinatorial data.
- Energy challenges often operate at time (ns – decades) and system scales (hundreds of millions of devices and sensor data streams) that preclude data aggregation and centralized training or inference. AI systems must be able to balance semiautonomous training and inference with coherence.

01. NUCLEAR ENERGY

To remain competitive in the electricity generation market and attract investment, nuclear power must embrace AI technology and innovation. As other market sectors adopt this technology, Nuclear Energy (NE) risks becoming less competitive. AI has the power to transform industries, so it follows that plans for the adoption of AI need to be on a commensurate scale. The approach in NE is to define grand challenge problems, those problems that are intractable using existing methods and whose solution will significantly alter the economics of the design and operation of nuclear systems. A grand challenge problem spans multiple disciplines and cannot be solved by conventional methods. The power of AI for solving such problems lies in its capacity to simultaneously countenance multiple system characteristics while incorporating both data and physics models and to do so on a scale not humanly possible. That is the setting considered for the nuclear energy space.

1.1 Grand Challenges

The lifecycle of a nuclear reactor is composed of multiple phases, each associated with activities that involve different skill sets, as shown in Figure 1-1. Each skill set is grounded in an engineering or science discipline with a knowledge base matured through decades of operational experience and documented in various formats (e.g., manuals, data sheets, textbooks, etc.). Although most of those activities are performed independently, the skillsets required are multidisciplinary. By seamlessly managing and coordinating these couplings, a substantial reduction in costs compared to existing expenditures for developing and deploying nuclear energy can be achieved [1]. In the recent commissioning of Generation III reactors, significant delays and cost overruns were encountered [2]. Some of the delays resulted from construction beginning before the design was completed [3], which could be mitigated using AI technology developed through the FASST initiative. These interdependencies and the challenges that they present are eminently addressable using AI. While a team of individuals could, in principle, maintain an exacting knowledge and awareness of the complex interdependencies in Figure 1-1, the task is challenging, both in terms of the expanse and depth of the information and factors such as succession planning and individual bias, all of which combine to test the limits of human cognition. AI offers an essentially limitless capability to store knowledge and the ability to recognize connections across disciplines where subject matter experts are inherently limited [4]. Three challenge problems have been identified where the power of AI/ML can potentially best what human teams might deliver.

CHALLENGE 1: ACCELERATING THE LICENSING AND REGULATORY PROCESS

The deployment of advanced nuclear reactors in the United States, crucial for achieving our clean energy goals, faces a major hurdle: a slow, expensive, and convoluted regulatory process. From design and construction to operations and eventual decommissioning, every phase of a nuclear reactor project undergoes rigorous scrutiny from the regulator, who is charged with providing reasonable assurance of adequate protection of public health and safety [5]. Moreover, the currently mandated process to obtain a construction permit and operating license for a new reactor in the United States can drag on for 5+ years, sometimes even decades if including preapplication engagement by the licensee, while incurring costs that can escalate to hundreds of millions of dollars.

For example, the most recent approval of a NuScale US600 Small Modular Reactor, with a rated thermal output of 160 MWt and electrical output of 50 MWe, was received after 8 years of preapplication engagement and a subsequent 6 years of a formal review of the application [6]. The company had to invest more than $500 million and 2 million labor-hours to prepare its licensing application, which encompassed a staggering 12,000 pages, 14 separate topical reports, and more than 2 million pages of supporting documentation for U.S. Nuclear Regulatory Commission (NRC) audits [7].

Furthermore, the current regulatory process, designed and evolved for the traditional light-water reactors, may not adequately account for the unique features, design innovations, and safety considerations pursued for advanced reactors [8]. Additionally, regulators have a need to acquire new subject matter experts (SMEs) and expertise on technical issues beyond their current scope of understanding the traditional light-water reactor fleet. New advanced reactor designs would introduce technical aspects that are largely unfamiliar to the reviewing staff, potentially increasing the number and frequency of requests for additional information and therefore, significantly delaying regulatory decision-making.

The current excessively prolonged and expensive licensing approval process will act as a significant barrier to entry for new companies developing the next generation of designs and innovative technologies [9], ultimately hindering the development and deployment of advanced nuclear reactors in the United States and adversely impacting the society’s clean energy ambitions and set goals.

Emerging AI technology, particularly the multi-modal LLMs, offers a powerful solution to these challenges. Trained on vast datasets of scientific literature, technical documents, and

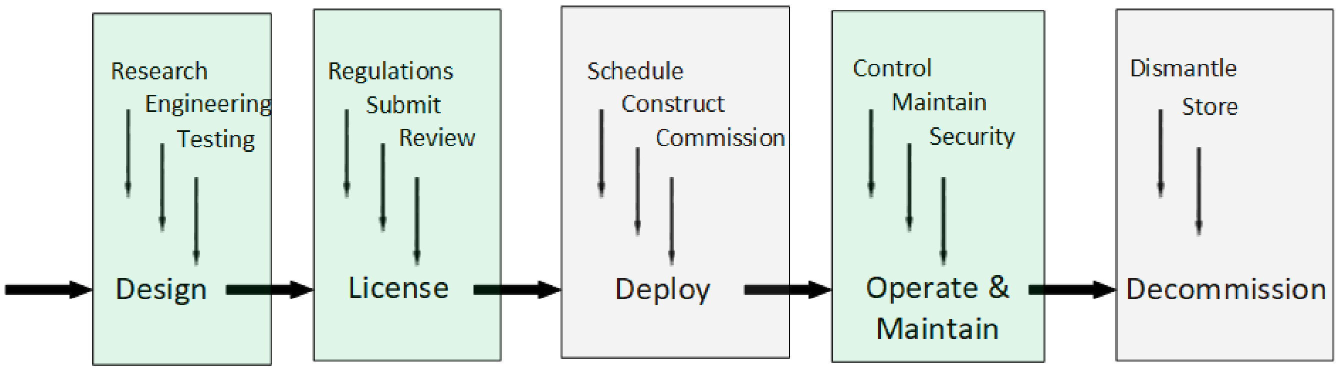

Figure 1-1: Cradle-to-grave lifecycle for a nuclear facility. Green denotes those phases and associated activities selected for transformational change through AI/ML.

operational data, LLMs can acquire remarkable capabilities that can substantially streamline and expedite the nuclear regulatory licensing and compliance process and make it much more cost effective for both the licensee and the regulator. By implementing LLMs as "virtual SMEs," the regulator can free up staff time for more critical tasks, improve communication, and prioritize safety by identifying risks earlier.

Dedicated public foundation LLMs can be developed, which are meticulously trained on curated datasets of publicly available information for advanced reactors that are being pursued in the United States. Such datasets would encompass resources from the U.S. Department of Energy (DOE), the NRC, broader scientific literature, and even data available from decommissioned reactors for operational insights. Such a foundation model would serve as a shared resource accessible to both regulators and applicants. Its capabilities could be further augmented through fine-tuning it with controlled, proprietary, or application-specific information. This allows the foundation model to cater to specific licensing cases or address unique safety issues, leading to enhanced confidence and more quantitatively accurate findings [10].

Once the AI foundational model is qualified and accepted for use, such a foundation model could have significant positive impacts in:

- Automating repetitive tasks: Handling the time-consuming burden of document review, information retrieval, and processing the reasoning of safety arguments; and significantly reducing the time and manpower required for reviewing applications.
- Bridging the communication gap: Translating complex technical safety arguments into relevant insights and fostering better communication between the regulators and applicants, which leads to faster resolution of ambiguities and streamlined interactions.
- Proactively identifying risks: Analyzing vast amounts of data from existing reactors and recorded historical events, pinpointing potential safety risks specific to novel designs or unique features, and enabling proactive mitigation strategies.
- Applying risk-Informed regulations: Analyzing existing regulations and identifying inconsistencies or gaps, facilitating the application of flexible and adaptable risk-informed performance-based regulatory frameworks specifically tailored to advanced reactor technologies.

The nuclear regulatory licensing and compliance process can be dramatically transformed by leveraging the power of LLMs, particularly a public foundation model. This transformation will significantly reduce time and cost, paving the way for the accelerated deployment of advanced nuclear reactors and a sustained clean energy future.

CHALLENGE 2: ACCELERATING DEPLOYMENT

Nuclear energy currently accounts for approximately half of all clean energy electricity generation in the United States [11]. Many of the current fleet of nuclear reactors were built decades ago. In fact, the average age of a nuclear power plant is 42 years old [12], whereas they were designed to operate for up to 40 years. Service beyond this lifetime leads to accumulated component damage and the need for more frequent maintenance. The DOE Loan Programs Office (LPO) estimates that the "United States will likely need 200 gigawatts of new nuclear generation by 2050 to meet national decarbonization targets" [13]. Even if all 200 GW of generation are fulfilled solely by large reactors, reaching this level of output would require the design and deployment of hundreds of new reactors over the next ~25 years. More likely, a combination of large, small, and microreactors will be used to meet this generation need.

The study, "Incorporating Digital Twins In Early Research and Development of Megaprojects To Reduce Cost and Schedule Risk," analyzed the benefit of digital engineering and digital twinning technologies as applied to nuclear power plant design and construction. It found a ~21% reduction in the probability of schedule delays [14]. Moreover, this study was authored prior to the release of new generative AI tools such as ChatGPT [15], which can serve as an adjunct to the design process. LLMs such as ChatGPT have already made inroads aiding in human–other endeavors [16] [17].

The design and deployment of new nuclear reactors are considered megaprojects as their budgets typically surpass $1 billion. Additionally, the time to design and deploy new nuclear reactors is expected to exceed 10 years. Of this schedule, approximately half of that time is spent in studies, licensing, and design activities [18]. Generative AI and digital engineering technologies (digital tools and software used to design, build, and analyze engineering systems) could dramatically reduce the time and cost prior to construction and reduce the probability of errors during the construction phase.

A new generative AI tool that can design a nuclear power plant could perform many key functions. AI models could autonomously generate the outlines, descriptions, and key artifacts needed early in the nuclear power plant development lifecycle to support environmental, stakeholder, and engineering document development. Furthermore, computer-aided design (CAD) drawings can be automatically developed from stakeholder input. Importantly, this AI-generated output can be validated with existing national laboratory–based, high-fidelity, multi-physics tools. These tools, representations of the laws of nature, can provide a cross-check on the physical reasonableness of an AI-generated design.

AI can potentially reduce future power needs by optimizing the planning and deployment of power generation. Site selection requirements may also be optimized using AI, such as regarding space requirements, local and regional ordinances, and available geographic landscapes, such as the amount of water needed to operate efficiently.

Using AI in the design and deployment process, it is possible that hundreds of billions of dollars could be saved during the design, development, and deployment of 200 GW of new nuclear capacity. It is estimated that a “well-executed first-of-a-kind nuclear construction project is ~$6,200 per kW” [19]. Given the 200 GW needed, this could represent a total cost of almost $1 trillion. Digital twins and AI can reduce delays by ~21%, potentially saving hundreds of billions of U.S. energy development dollars by 2050.

CHALLENGE 3: FACILITATING AUTONOMOUS OPERATION AND MAINTENANCE

The staffing requirement for the operation of a nuclear power plant in the U.S. presents a challenge compared to other electricity-generating sectors [20]. A modern 1100 MWe natural gas plant has 35 employees, a relatively low staffing requirement attributed to the use of data analytics and automation [21], which compares with 800 at a comparably sized nuclear site [22]. Given recent developments in AI, the opportunity exists to rework the human resource allocation problem that puts nuclear energy at a disadvantage. AI can substitute for human presence for a wide range of tasks in a nuclear plant.

The objective is to move toward the *semi-autonomous operation and maintenance* of a nuclear facility. That is, using AI will minimize the need for direct human involvement by simultaneously carrying out complex cognitive tasks involving many engineering disciplines [23]. The unattended mode of operation introduces the possibility for a new level of operational efficiency with the possibility of coordinating and managing monitoring [24], control [25] [26], and maintenance [27] activities across multiple plants at a single remote center. One envisions semi-autonomous operation where a plant meets its operating objectives through monitoring [28] and control [29] tasks performed by AI to deliver the electric power demanded. AI can assist in explaining a fault diagnosis to mitigate complex system failures by leveraging physics-based knowledge [30] [26].

This new paradigm can be regarded as the analog of the *edge computing* problem, defined as having physical computers at the edge, where the AI performs these lower-level tasks locally at the plant. Higher-level tasks are outsourced to the remote center where the results of the lower-level “edge computing” tasks provide input to tasks for maintenance scheduling, supply chain management, and issuance of electric power demand.

The concept of a remote center powered by AI admits a higher level of autonomy, that of managing and coordinating a collection of nuclear and other generating assets. This problem exists where the grid interfaces with individual generating assets. AI has a role to play in this setting in scheduling these assets to ensure that electricity demand at the grid level is met in a manner that is optimal for cost and reliability. This coordination, which involves the collective management of generation, plant outages, and maintenance activities, is a problem that presently requires reserve capacity to meet scheduled and unscheduled disruptions to generation. AI, with its ability to analyze and predict with greater speed, precision, and awareness than a human, can improve economic margins by reducing the need for reserve generation. All the while, AI facilitates human understanding of the state of the individual plants and the integrated plant system it manages.

The economics of performing maintenance improves by using AI to support several tasks [27]. Physical activities do not go away. Rather, algorithmic activities are substituted in place of human cognitive activities. AI can monitor equipment performance continuously, predict potential malfunctions, and conduct maintenance before failures occur, improving plant reliability and safety. AI can be used to optimize nuclear power systems and plant operations, reducing downtime, improving efficiency, and increasing the safety and reliability of the plant. AI can also analyze large amounts of sensor data and other plant data [31] to identify patterns, trends, and anomalies [32] [33] that signal potential problems or maintenance needs so they may be corrected before an outage or failure occurs [34] [35].

The workforce problem that becomes solvable with AI goes deeper than just improving the efficiency of deployed human resources. Experienced nuclear plant operators are scarce [36]. Even if there is success in accelerating all of the upstream processes that lead to many new plants being built, there is a looming shortage of qualified nuclear plant operators [37]. Operators are scarce because it is a tough job, and so are working conditions. Extensive certifications are required [38], and often, plant sites are in remote locations, which limits the labor pool from which operators can be drawn. Remote monitoring enabled by AI equates to lower labor costs, better safety, and greater workforce sustainability.

Having presented the value proposition, the focus turns to how AI can be used to this end and how it should be deployed. AI can see connections in data where the human is challenged, given the size and dimensions of the data and information. The key is to harness that unique capability to complement the human and deliver a solution that coheres across the breadth and depth of the engineering disciplines involved in an operating nuclear reactor.

1.2 Advances in the Next Decade

With the advancement of AI, it is possible to containerize all that mankind has learned about nuclear energy to make it more widely accessible, while also critically restricting information appropriately. With decades' worth of accumulated data and knowledge, it is possible to design one AI model that can capture public and private information (including restricted domain) and perform all activities over the life cycle of a nuclear plant. The AI model feeds the data in various formats, including text, tables, figures, images, video, and experimental or operational measurements, and consolidates the available human history of nuclear energy knowledge in a single model. This model could perform any of the nuclear reactor lifecycle functions, such as designing a new reactor while considering constraints from operations, deployment, commissioning, etc. It will be able to modify and optimize various activities as new findings are obtained by using the suite of development tools developed under the general initiative, eventually becoming a nuclear energy expert with a knowledge base that exceeds the capabilities of a human.

Developments are needed in five areas to advance this proposition, from concept to delivery. Below, we assess the current status, and in Section 1.3, we describe how to accelerate the needed developments.

ADVANCEMENT 1: FORMULATE A LEADERSHIP COMPUTING CAPABILITY ECOSYSTEM

The AI4E initiative is to deliver AI hubs that can solve grand challenge problems in energy. It envisions an ecosystem of high-performance computing (HPC) capabilities that supplants the current collection of individual machines, each deployed as a stand-alone computing resource. The current generation of stand-alone HPCs built on networked graphical processing units (GPUs) would be transformed into a next-generation network of coupled HPC machines, with applicable edge computing devices for downstream tasks. The result would be an increase in computational capability over what exists now as stand-alone machines are an underutilized capability. An objective is to solve problems in nuclear energy that are presently beyond the reach of any single HPC machine.

To achieve this advance, high-speed data pipes and data centers are needed to facilitate communication and algorithms to coordinate tasks and to seamlessly exchange data among HPC machines.

ADVANCEMENT 2: EXPAND ON BASE FOUNDATIONAL MODELS TO INCLUDE NE

Nuclear energy, along with the other four topics – power grid, carbon management, energy storage, and energy materials – have their own specialized domain knowledge which is not well represented in existing foundation models. Existing models were created with commercial applications in mind and so target a different user than the science and engineering subject matter expert that the AI for Energy initiative aims to enable. So, in general, the existing foundation models have not been trained on the knowledge that is fundamental to our applications.

A foundation model suitable for nuclear energy must include the specialized engineering and science data and information that subject matter experts have developed. That time stretches back to the genesis of the peaceful use of nuclear energy in the 1950s, and it includes technical reports, literature publications, and all manner of archived materials related to the peaceful use of nuclear energy.

Further, the foundation model must be capable of representing the time-varying nature of nuclear systems whose dynamic characteristics are essential to operation and safety [39]. However, the typical LLM-based models are not suited for capturing this behavior. Additionally, there is insufficient data at large to sufficiently populate this space adequately for training a model.

One solution is to complement the foundation model with fundamental physics-based information cast in a form used to represent the laws of nature [40]. For example, in predicting the operating behavior of a nuclear reactor core, equations that describe heat generation and neutron multiplication are solved for the reactor's state. So, the foundation model will include such equations and their solution data as generated by a simulation code that solves these equations [41]. Further, if the problem involves sensor data, then this data must additionally be included [42]. Incorporating physics-based models, which represent the laws of nature, into the foundation model, in combination with sensor data can, in principle, result in a more reliable and robust model than found in a purely data-driven model, as is demonstrated in [40].

ADVANCEMENT 3: ENSURE THAT THE AI ENABLING TECHNOLOGIES AND TOOLS ARE AVAILABLE FOR NUCLEAR

The current development of AI for nuclear is application-oriented and confined to the needs of subject matter experts without regard necessarily for what a larger enabling ecosystem might look like [43]. New tools are needed in this envisioned larger cross-disciplinary space [44].

Nuclear energy has unique security and safety issues that are not adequately addressed by current AI environments. Models must operate in software frameworks and data infrastructures that support large-scale workflows, all with physical security, cybersecurity, and operational security in mind. Some specific requirements are listed here.

1. A software framework that supports workflows and the inclusion of physics models that constrain solutions to those physically realizable.
2. A basic infrastructure that is sound. If a system using AI performs a critical function, that function should not be compromised should the AI fail for whatever reason.
3. A means to judge what is a permissible use of AI in a particular application from the standpoint of security and safety and what are needed layers of protection.
4. A way to enable transfer from private companies' reactor data that may be proprietary and to create appropriate assurances.
5. A means to qualify the AI with respect to reliability, robustness, security, and utility when it is drawn from all types of information.

ADVANCEMENT 4: PROVIDE FOR TESTBEDS FOR VALIDATING AND EVALUATING AI METHODS FOR NE

To realize the inherent power of AI systems, it will be necessary to train on a platform with the richest scientific datasets. With the high standard for AI model qualification in the nuclear energy domain, this platform ideally would involve a physical testbed. A testbed provides a direct means to address issues associated with AI interacting with a physical plant with its attendant safety and operating performance objectives. For example, the value proposition of AI for nuclear energy will almost certainly involve improving the efficiency of plant operations and maintenance of equipment, something whose qualification can be explicitly addressed using a physical testbed.

In one approach, AI could be exercised on a semi-scale engineering facility, such as that for testing nuclear plant components. Ideally such a facility would support operation outside of "normal" to test the various contingencies that the AI would need to have built in and include digital components to enable a comprehensive environment for testing (for instance, as described in [45]).

As is the case with all nuclear industry software deployed in operations, earlier stage development requires shakedown tests on an engineering simulator. The development then progresses to use for training nuclear plant operators and for testing operating procedures.

Other approaches to accelerate initial qualification are to train AI on a history of data from commercial reactors and see how it performs versus that history. This approach addresses such questions as: does the AI run a facility better than the humans did and how close does it get? Such approaches also point to the need for rich data sets and an associated data management infrastructure that complements testbeds.

ADVANCEMENT 5: INTEGRATE EXISTING INFRASTRUCTURE TO TRANSFORM INTO A NATION-WIDE RESEARCH RESOURCE

To create unprecedented data and experimental resources for advancing AI research in the nuclear domain, we can begin by integrating the knowledge and infrastructure expertise across the DOE complex.

In the knowledge domain, many researchers in NE see publishing their work as the end game without necessarily pursuing synergies across other NE subject matter domains. Instead, a new mindset that aims to spur collaboration would better fit an environment where AI is expected to house all that mankind has learned about nuclear energy. An inter-Office consortium model where subject matter experts are brought together from across DOE Offices to solve a challenge problem could facilitate this.

In the infrastructure domain, work could start in a bootstrap fashion beginning with the collection of related systems and the training of each independent of the others; and then later, when the AI infrastructure has sufficiently evolved/developed to support integration, they are trained together.

Regarding facilitation, DOE needs to provide incentives for sharing data and collaborating and provide DOE-sponsored mentorships.

1.3 Accelerating Development

1.3.1 CENTRALIZING DATA AND FACILITATING ACCESS

While data is abundant, its format, availability, and provenance are highly inconsistent and cover a broad range of scenarios. Therefore, a critical first step is to create a comprehensive data repository and develop an ecosystem around it. This ecosystem should utilize the DOE infrastructure, which offers one of the most powerful computational capabilities in the nation and is well-positioned to take on this challenge – see two advancements in Section 1.2, *Formulate a Leadership Computing Capability Ecosystem* and *Integrate Existing Infrastructure to Transform into a Nation-Wide Research Resource*. It should integrate the knowledge, data, and resources available across the DOE complex and solicit participation from the private sector. Power and communication infrastructure should be considered as a supplemental but key part of a data pipeline. A dedicated infrastructure task team is needed to develop this ecosystem. Furthermore, given the highly diverse nature of the data, a dedicated data task team is needed to develop and implement a strategy to collect for data collection and organization.

1.3.2 NEW METHODS

A significant and essential component of nuclear energy data and knowledge is manifest as the output of computer codes that represent the physics of a nuclear system. AI needs to access this information if it is to have its own internal and accurate representation of the physical system. New methods based more on the models that generate the code output would better serve as a canonical representation [40], especially considering the multitudinous and diverse nature of the spatial and temporal resolutions.

With their physical models, these computer codes make predictions of physical quantities in time whose evolution is not directly observable in measurements. But they also yield a time-integrated behavior to produce a measurable observable, such as mechanical damage to a nuclear structure. Methods are needed [46] to meld these observables, as found in experiment and industry datasets, with the aforementioned models for enhanced predictive power.

Additionally, there are hybrid data forms that involve qualitative and quantitative descriptions and inhomogeneous data (i.e., a combination of text, time series, images or figures, etc.). Current methods have only targeted subsets of those characteristics. The performance of the AI in terms of reliability, robustness, and validity hinges on providing a comprehensive description of the model's training.

With the increasing amount of data and knowledge to be captured, these proposed new methods need mechanisms to understand the evolution of knowledge and possible conflicting insights and findings. They also need the means to understand when insufficient data is provided, such in first-of-a-kind designs, and to decide and highlight areas of future research to close scientific and engineering gaps or perform self-guided simulations using available tools to close any gap.

1.3.3 NEW TYPES OF MODELS, NEW TOOLS, AND NEW WORKFLOWS

The methods should be able to convert their knowledge into surrogate models and tools to meet functional requirements in every phase of the mentioned cycle. Those tools can be self-validated by high-fidelity tools and self-tuned as new information becomes available that either confirms or refutes its comprehension or predictions of certain phenomena. They can also be shared with a human counterpart for additional validation and as a tool to advance science and technology.

1.3.4 CONNECTIONS TO EXPERIMENT, SIMULATION, AND THEORY

In parallel to data collection and methods development, a test platform is needed to evaluate and tune the models and tools before their deployment. The methods should be able to mine through the data for existing validation data and experiments before suggesting a target validation experiment in the test bed. The test bed design should be broad enough to cover all phases and aspects of nuclear energy (Figure 1-1). It should replicate the tools and processes performed in every stage of a reactor's development and deployment. Given the depth of the test-bed role, it is envisioned that it will be distributed into multiple facilities that compose the main test bed and leverage existing DOE infrastructure when available.

To speed up the testing and validation of models or even model components, it is likely that experimentation on purpose-built testbeds will need to be conducted. Physical implementations allow for quicker development through more efficient validation of software models as potential problems can be more easily identified and tested.

1.3.5 SCALE OF MODEL BUILDING AND COMPUTING NEEDED

Advanced reactor developers have lamented the wealth of experimental data that reaches back to the early days of the development of the peaceful use of nuclear energy — but that is largely inaccessible. On an individual company basis, they do not have the resources to retrieve and order the data in a form ready for use.

There is, however, a scenario under which HPC and LLM technologies supported by federal funding can be leveraged to address this problem and provide an even richer solution than what was imagined by these developers, which was before the advent of ChatGPT.

The power of LLM to capture enormous troves of data and search out cross-data connections and relationships on a scale that is almost beyond human-like capability has been demonstrated in the private sector [47]. The largest HPC machines at the national laboratories have a computational capability of comparable scale. They should be used to create LLMs that are analogous to those in the private sector but serve the public good. Making all engineering and scientific data produced to date available in an LLM would serve the specialized needs of the nuclear energy community. The case in point is accessibility to all nuclear energy records, as mentioned above.

1.3.6 SCALE OF TEAMS NEEDED TO HAVE CONFIDENCE OF SIGNIFICANT PROGRESS

Given the scale of skills and effort required to collect all relevant nuclear energy data, curate and prepare the data, label it when needed, process it, and structure or model it, a team needs to be assembled with a skillset representative of the various Figure 1-1 phases of nuclear reactor development. The team should be familiar with the types, locations, forms, validity, fidelity, and depth available in both the public and private domains and would interface with the private sector to discuss the expectations and benefits of accessing the data.

A separate methods-focused team would also need to be assembled with an understanding of state-of-the-art AI models and how they are used. The team would be exposed to the nuclear energy acquired data and will develop a plan and execute it to achieve the objectives discussed earlier.

A third team will be assembled to test the models developed. This team would be composed of independent developers and potential users. Initially, they would need to design the needed testbed requirements and survey potential facilities that can meet parts of the testbed objectives. The team would also integrate the various roles and connect to create a validation and testing process and infrastructure. This team will also work with the methods and data teams to design benchmarking and evaluation scenarios and how they would be incorporated into the models being tested.

Given the extensive reliance on information technology (IT) infrastructure to establish the discussed ecosystem, a dedicated team is proposed to establish the data storage, data analysis, and communication pipeline infrastructures and implement the needed safeguards and cybersecurity measures. This team will also decide how to leverage external and internal IT resources and the optimal means to achieve that.

The four main teams (for data, methods, testing, and infrastructure) would be supported by essential organizations, such as legal, to ensure that data sharing is compliant with laws and establish agreements with private industry stakeholders when needed.

1.3.7 DEPLOYMENT OF MODELS AND APPLICATIONS

As a new and relatively untested technology with few time-proven applications, AI and its deployment best proceed in a bootstrap fashion. Supervised learning in the initial stages provides a trained model with well-defined boundaries of applicability and validity. As confidence in an adjacent and parallel reinforcement learning model is gained, NE users can gradually transition to the latter (trained model). So in this approach, the former is accepted as the initial operational solution while the latter is carried along for continued development and qualification to eventually become the accepted solution. Or more generally, different elements can be enabled and change over time, leading to progressively greater autonomy in training and adaptation to a changing environment [10].

AI systems need to be routinely monitored and adapted to a changing environment. In one existing deployment in the nuclear industry [48], new data becomes available periodically, is uploaded to the cloud [16], and models are updated to maintain concurrency.

1.3.8 CRITICAL PARTNERSHIPS

The potential benefits of integrating existing infrastructure across the national laboratories into a single, highly effective resource were described in Section 1.2.

Across the different Offices of DOE, there is the need for partnerships. Each Office brings with it a unique subject matter domain. Bringing all of this knowledge under one LLM model is critical to the advances sought under the grand challenge problems. The different Offices need to collaborate on all aspects of building an inclusive LLM model including data curation, data formatting, model architecture, training, and deployment.

1.3.9 RISKS, SAFEGUARDS, AND SECURTY REQUIREMENTS

If this model is to develop and deploy reactors and then operate them, it needs to be secured, qualified, credited, and validated according to the industry’s norms, policies, regulations, and laws.

Modern artificial intelligence approaches are stochastic, meaning the system is intentionally designed to be able to react in unpredictable ways to create novel output. This aspect can be adjusted and is referred to as the model “temperature.” This design inherently means that security and safeguards measures must be put in place to account for the unpredictable behavior of a given model. Considerations specific to nuclear (regulatory, security, etc.) may require development of approaches for explainable and trustworthy AI and qualifying the methods for nuclear applications, and further research will be needed to adapt AI approaches to account for these concerns.

Experts in AI will need to be aware of the potential threat vectors that can be used against the developed model so they can incorporate security into the design from the ground up, and also build in cybersecurity plans throughout the development lifecycle to prevent misuse of the training data and vulnerabilities in the model, as well as safe operation throughout its lifecycle.

1.3.10 WORKFORCE AND TRAINING REQUIREMENTS

A foundation model capable of accelerating the deployment of nuclear power facilities will require experts in many subject areas that require extensive education in fields such as algorithms, uncertainty analysis, process engineering, networking, databases, computer communication, visualization, human factors, facility operations, and more. With these positions in high demand in many fields due to the recent sensationalism on large language models, it is imperative to identify and develop methods to attract and develop talent within our academic institutions, universities, and national laboratories. A sponsored mentorship program in AI is needed for those disciplines with the greatest demand for labor and that are expected to have the highest growth rates. A study could be performed to identify those areas.

1.4 Expected Outcomes

A solution to the grand challenge problems and the development of associated methods and software will provide a transformational national capability while leveraging the knowledge, skills, facilities, and resources based at the national labs and universities. For these communities, a common resource platform will be needed for development and validation tools/training to streamline and maximize AI benefits.

The goal is to put foundational tools in the hands of advanced reactor developers for advancing the performance of nuclear systems and putting these tools into the hands of regulators for their acceptance for use in safety-related applications. This effort will enable the ultimate goal of optimizing the development, deployment, and operation of nuclear power generation using AI.

The timeline is 10 years to establish a foundation for AI methods where the unique capabilities and potential are recognized and adopted by advanced reactor developers. In the interim, there may be an advantage to proving and demonstrating AI technologies in the existing reactor fleet or at DOE facilities.

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02. POWER GRID

The energy system, which runs the world's economy, is becoming increasingly complex and undergoing a transition not seen since the advent of electricity over 100 years ago [1]. Grid balance and stability now rely on digitized control and increased reliance on communications, information exchange, and data. The amount of smart, distributed technologies is increasing exponentially through the deployment of electric vehicles, rooftop photovoltaics, local energy storage, and smart building technologies. Additionally, there is an increasing amount of electrification and significant changes in the primary energy mix to more variable and distributed renewable energy technologies, such as wind and solar. This transition, which is required to decarbonize the energy sector, is happening at an unprecedented speed and scale in the energy sector [2], changing from the known generation and demand patterns that were used as the basis for managing the grid. These changes impose a level of uncertainty in operating distributed energy systems, requiring higher spatial and temporal resolution of monitoring, forecasting, and control. Increasingly, parts of the grid are managed by multiple owners and jurisdictions imposing challenges in data sharing, planning, and operations. There is also a level of uncertainty about how these emerging, new kinds of power will be managed in the future; and, as increasing parts of the grid are under multiple owners and jurisdictions, this situation creates an ever more uncertain future in planning and operations. While our knowledge about how to handle complex systems is continually increasing, artificial intelligence (AI) is starting to show promising solutions for making the complexity of the data-rich future grid more manageable.

2.1 Grand Challenges

Herein we describe three grand challenges in the transition of the Energy System that AI can help solve over the next decade (Figure 2-1):

- Realizing proactive, real-time energy system operations
- Building cyber- and all-hazards resilient and secure energy systems
- Designing and planning a 100% clean electricity system by 2035

Figure 2-1. Grand Challenges for Power Grids

CHALLENGE 1: REALIZING PROACTIVE, REAL-TIME ENERGY SYSTEM OPERATIONS

The growing complexity of the grid is making it increasingly difficult to operate efficiently. Operators are expecting orders-of-magnitude increases in the number of smart devices interconnecting with the grid [3] by 2050. Technologies such as electric vehicles and chargers, smart buildings and appliances, roof-top photovoltaics, large-scale solar and wind plants, energy storage, and smart meters are all being rapidly deployed because of relatively low costs and the ability of these devices to increase customer satisfaction around energy use. This significant paradigm shift from a centralized system of large plants providing the bulk of electricity to a more distributed generation model with resources sited near customers — as well as the increased intelligence required to support smart loads — will strain the ability of grid operators to maintain reliable operations. The need both to process vast amounts of information, measurements, and data to better estimate the state of the grid and to create forecasts to proactively improve grid operations continues to grow. In the future, grid operation will need to estimate load composition and settings at the customer level and compute many more supervisory control signals to be tracked by the distributed resources, probably by factors of 100 to 1,000. Solving the resulting estimation and control problem in a timely manner under the uncertainty of environmental states and system settings (the latter needed to estimate the flexibility potential as well as transient response) requires the latest advances in AI techniques, which can analyze vast amounts of information, identify patterns, and create forecasts in real time [4].

Revolutionizing grid operation by providing support for the proactive operation and predictive online control of the power grid to achieve improved efficiency, reliability, and resilience will require new foundation models. Proactive operation will be enabled by four capabilities: (1) handling the massive amounts of real-time measurements at different temporal and spatial resolutions such as phasor measurement units (PMUs), point-on-wave sensors, supervisory control and data acquisition (SCADA), advanced metering infrastructure (AMI), etc. (the measurements, including both electrical and environmental information as well as states of other energy infrastructures, will be fused and curated for different purposes); (2) increasing the data-driven predictive capability at timescales ranging from sub-seconds and seconds for the incipient failures and dynamics and stability assessment associated with the inverter-based resources (IBRs) and conventional generators to short-term (hours and days) locational forecast of the correlated renewable generation and demand and impacts of hazardous weather events; (3) enabling the prognosis, diagnosis, identification, and locating of disturbances and the online prescription of optimal control design for stabilization and service restoration based on the combined information of the grid's real-time and predicted operational conditions; and (4) enabling AI-based sub-hourly energy scheduling and dispatching for optimal operating points of the power grid based on the grid status and predictive capabilities of generation, demand, and stability margin.

CHALLENGE 2: BUILDING CYBER- AND ALL-HAZARDS RESILIENT AND SECURE ENERGY SYSTEMS

The nation's aging infrastructure, extreme weather events, and the grid's increasing complexity are impacting robust management of system reliability and resilience; meanwhile, our reliance on electricity has been increasing for everything from transportation to communication and home appliances [5]. Additionally, cybersecurity vulnerabilities exist across all digital components of the grid. All hazards (human-made, cyber, and natural threats) are increasing and driving broad disruptions across the U.S. Harnessing AI provides the best opportunity to achieve a cyber- and all-hazards resilient and secure grid by reducing blackouts and brownouts and ensuring that all communities have access to affordable, reliable, and clean electricity.

Traditional approaches like grid modeling and planning are not enough to protect against complex and coordinated threats/attacks. AI and data fusion from disparate data sources can be effectively used to detect and mitigate complex disruptions (e.g., winter storm) anomalies in ways that existing methods or human operators are not able to do [6]. A foundation model using sensor data with other intelligence information could diagnose the cause of the impairment and neutralize its effect rapidly, increasing resilience by providing real-time prevention and mitigation of disruption due to extreme events, whether natural or human caused. AI could diagnose and generate real-time recommendations for actions that should be taken in response to attacks, failures, or other impairments. Malevolent actors will employ AI to find and exploit unknown vulnerabilities, while grid operators will also need AI to find and fix vulnerabilities before they can be exploited. AI models can also be used to cost-effectively inform emergency response and resource needs at the community level during extreme weather events and/or power outages, which makes them especially useful for disadvantaged communities.

CHALLENGE 3: DESIGNING AND PLANNING A 100% CLEAN ELECTRICITY GRIDS BY 2035

Achieving a 100% clean electrical grid by 2035 and all domestic energy use by 2050, while maintaining today's reliability and perhaps improving it considerably, will require multiple technological leaps. Industry operators need to plan, site, review, and permit unprecedented amounts of generation capacity as well as extensive transmission and distribution infrastructure. These needs are complicated by the fact that these reviews and approvals are spread across thousands of federal, state, and local jurisdictions. One of the inherent difficulties in the designing and planning process is understanding the languages used among different entities, which can be facilitated and streamlined by using large language models. As planning, siting, and permitting actions increase with growing amounts of variable generation, operators will need significantly more accurate weather and climate forecasts to understand the impacts on generation and consumption, while still being able to balance supply and demand on multiple time scales at the required reliability. The declining proportion of dispatchable resources, reducing both the controllability and inertia of the system, will require greatly improved load estimation approaches, in combination with the deployment of smart grid and advanced technologies such as storage. Operators will not be able to address the complexities and accuracy margins of forecasting, planning, and operating reliably under such uncertainty without artificial intelligence technology.

In fact, AI can change the planning paradigm for the future power grid by providing fast and efficient surrogates, high-fidelity scenarios, and stochastic optimization schemes for large-scale integrated energy systems. AI-based, multi-fidelity surrogate models for dynamic components need to be designed, built, and integrated to implement a large-scale dynamic emulator with uncertainty quantification for the planning of the power grid. The AI-based or hybrid grid emulator can be used to replace the existing numerical methods-based simulation tools such that steady-state and dynamic contingency analysis of utility-scale systems can be performed both online and offline. Moreover, improved long-term planning can be achieved only by using more realistic scenarios projected for the planning horizon. Such scenarios could be developed using AI and historical data to account for both technological evolution and climate changes while quantifying the associated uncertainties.

2.2 Advances in the Next Decade

While AI holds great promise in this area, grid operations have a set of very specific requirements that AI, to date, has not been able to satisfy. Scheduling and dispatching activities need to satisfy very complex constraints, such as line and voltage limits, which are both coupled through power flow and have a very high number of dimensions (including safety). While this constraint can be formally addressed by a reinforcement training metric, the outcomes typically do not have the required accuracy (which is much more stringent in constraint satisfaction than in optimality). Moreover, the complexity of optimization algorithms tends to be different for this circumstance. Recently, significant progress has been made through embedded AI, which aims to capture a latent representation of the decision space combined with a projection over the feasible space [7]. Another difficulty concerns AI used in the loop when it concerns the stability guarantees of closed loop systems. Many AI methods (such as the ones trying to approximate the autoregressive maps of physical systems) typically lack the ability to preserve / guarantee stability because they do not rely on the same algebraic principles. Determining AI structures that intrinsically preserve stability (e.g., by ensuring monotonicity over certain variable ranges) is a crucial endeavor for ensuring their stable and safe operation in this area. To improve the system's reliability and resilience, any AI tools that are adopted will need to:

- Provide stochastic, robust design for a system operating under increased uncertainty.
- Predict vulnerabilities and biases at community and district levels considering equity, social-economic factors, and condition(s) of the infrastructure.
- Predict equipment degradation and failure so as to propose maintenance, repair, or replacement.
- Perform real-time event and disturbance classification, with online dynamic contingency analysis.
- Provide decision-support algorithms for predicting and preparing for rare and extreme events.

Maintaining the stability of the power grid is crucial to its reliability and security. It is important to note that, as many events are not foreseeable (such as wildlife and weather causing short-circuits), operators aim to have not only real-time stability but also virtual stability against events that have not occurred but might. Historically, this is carried offline on a limited number of scenarios, and conservative operational margins are prescribed (for example on intertie flow limits) to help ensure stability, resulting in both increased cost and reduced flexibility, and potentially, reliability. Thus, one advance that is highly needed is to provide a sharp stability margin in real time, which is fundamentally a complex mapping between the system state and its transient characteristics and is thus ideally suited for real-time calculations. For example, approximate synthetic energy functions are suitable only when there are small-noise limits in calculating stability [8]. AI-based energy functions have the potential to provide far more accurate and valid energy functions to obtain a sharper approximation of stability and security, thus reducing cost and improving flexibility. A related issue is that of rapid propagation of the state uncertainty through the transients, particularly in the context of preventing cascading failure and away from the large deviation/small noise approximation. An AI effort may vastly accelerate recently proposed ideas to use machine learning to approximate the Fokker-Planck equation [9].

In the power grid setting, using advanced large language models could help human teams converse with one another and remove ambiguity. Interacting as an effective human-machine team could improve the coordination between operator teams with varying skill sets, efficiencies, and expectations. This improved coordination may also become one of the most impactful benefits of natural language processing in terms of opportunity cost, because it affects organizations at all levels – especially grid operations and planning staff.

For foundation models to be used in high-consequence systems, we need a provable understanding of its bounds. For example, a significant challenge in predicting rare events is the issue of data disparity. This refers to the situation where there is a disproportionately low number of instances of rare events (positive examples) compared to regular events (negative examples) within the dataset. As a result, AI algorithms may develop a bias toward the more frequent case, leading to the overlooking or incorrect categorization of the less common event. Overcoming this bias will require new approaches so that foundation models can address scenarios beyond the "average" case to include different distributions, such as black swan events. New research is needed for explainable and trustworthy AI that is verifiable for safety and security. In order to improve cyber-physical security through AI's application, operators will require the ability to:

- Design our system around bad actors (moving target defense, robust design, etc.).
- Rapidly vet anomalous activity in broader contexts.
- Observe disparate data streams to assess the cyber-physical threat posture of the grid or other infrastructure.
- Autonomously detect network intrusions and physical asset attack posture.
- Identify vulnerabilities before they can be discovered by bad actors.

The area of weather forecasting and climate modeling poses a set of both important challenges and opportunities. The area is remarkable in that most of the data are publicly available and the physical processes describing its evolution are mostly known. The state space, however, is enormous; and the intrinsic chaotic behavior of this system results in the necessity of representing forecasts through probability distributions as opposed to point estimates. Many climate models are available to produce quality estimates of the distribution of atmospheric variables at scales of hundreds of kilometers; and while they are validated on a monthly or seasonal timescale, they generally produce hourly time series of the distributions, which is compatible with many of the tasks needed to carry out 2035 energy assessments. The energy infrastructure, however, interacts on scales of about 10 meters, such as at the scale of buildings, for example. Obtaining accurate distributions for atmospheric variables at a 10-meter scale and at subhourly resolution, as required for suitable characterization of renewable generation and demand. This is a grand challenge ideally suited to being addressed through an AI approach. At a conceptual level, the challenge is to create the map between climate-scale modeling (meshes of a few hundred kilometers, and every-hour time scales) and the target scales (10 m and a few minutes); as such, an AI-based endeavor could “crack the code” of this problem. Because most existing downscaling hypotheses assume this map to be stationary, at least starting from a sufficiently fine level, it can in principle be learned from existing data and applied to future climate simulations. We note that AI already had a stunning success with fourcastnet [10] when a Fourier Neural Operator trained with reanalysis data provided a forecast as accurate as one obtained through numerical weather forecasting but with 10,000 times better energy efficiency. In turn, it rapidly became the production forecaster of the European Centre for Medium-Range Weather Forecasts (ECMWF). The same approach can in principle be used with downscaling and would vastly improve energy efficiency.

2.3 Accelerating Development

NEW DATA

With respect to data needs — which implies data sharing among the hundreds of entities in the energy sector — substantial investments are needed in state-of-the-art data infrastructure that includes advanced sensing technologies, smart meters, secure cloud storage solutions, and data processing capabilities that can scale with demand. Automated tools for data cleaning and preprocessing, including anonymization, are essential to maintaining data privacy, data quality, error correction, and the ability to handle messy operational data sets of different spatial and temporal resolutions. Also, promoting interoperable data standards within the sector can dramatically improve the technical ease with which data are shared and integrated across various platforms and organizations. On the legal front, creating, motivating, and securing clear data-sharing agreements and mechanisms, including nondisclosure agreements (NDAs) and data access agreements, should be part of the proposed solution. These agreements must articulate the terms of data use, responsibilities, rights to modification, and redistribution, and must provide measures of confidence to the utilities and other entities for sharing proprietary or sensitive data [11]. At the same time, the data solution must ensure that practices are compliant with industry regulations, such as North American Electric Reliability Corporation (NERC) Critical Infrastructure Protection (CIP) standards.

For example, with the data that federal agencies need to comply with the National Environmental Policy Act (and related reviews like the Endangered Species Act, Clean Water Act, National Historic Preservation Act), there is little consistency in where or how the data are stored as well as incredible heterogeneity (which increases complexity) in the document structures themselves. For utility-scale wind and solar, there are perhaps 3000 relevant authorities having jurisdiction (AHJs). For devices such as battery storage, electric vehicle (EV) chargers, energy efficiency building codes, etc., there are ~28,000. Not all of them are fully digitized. Around 3,000 localities have ordinances and codes available through one of three or four aggregator services.

For each of the grand challenges described, many different types of data will be required:

- Geospatial geographic information system (GIS) information about grid data, including information about locations and types of critical infrastructure, land use information, aerial imagery, and other data.
- Data-driven, high-fidelity, black-box models of critical assets (e.g., inverters, relays) where vendors are gradually moving toward standardizing hardware and customizing software where possible.
- Customer behavior data to understand and forecast energy use.
- Historical climate/weather and outage data and staff logs for improving situational awareness.

Improvements in AI technologies could be substantially assisted with the gathering, organizing, and processing of the data.

NEW METHODS

Storage is a key component of a reliable future energy operations scenario driven by variable renewable resources, but it is not a panacea. There is a goal to achieve improved reliability in a future grid with far less control of the generation and reduced inertia requires extracting the maximum amount of flexibility from distributed resources and coordinating many more and smaller systems. It has been amply demonstrated that inverter resources can be driven to express both virtual inertia and storage functions, and this expanded flexibility is in principle usable to compensate for the reduction in dispatchability due to the retirement of classical generation [12]. Achieving an integrated solution across grid balancing areas, however, requires solving a gigantic state estimation, control, and optimization problem online. AI techniques are ideally suited to producing the coordination signals for all these resources to offer the transient stability and balancing the robustness needed to achieve improved reliability with the far fewer dispatchable resources available in 2035.

One of the key challenges in planning can be the inconsistent interpretation of the same requirement by different stakeholders. These interpretations may be motivated by drivers such as cost, revenue, policy, etc. A planning-tuned foundation model could be used to normalize these biases by training on the performance / restrictions of the stakeholders and to help the planners prepare a better "bare-bones" solution (a quick first draft) or negotiate more effectively on changes. For example, the next revision of a distributed energy resource interconnection standard may start with poll results from all the different stakeholders — which will then be fed into AI — to review and identify the sections that are likely to create the most/least conflict and then proceed from there. The first poll itself may be drafted based on the entire log from kickoff to final ballot to help identify the most crucial or comprehensive set of questions.

It should be emphasized that the chaotic nature of weather systems makes impossible the validity of point estimation; therefore, a*ny forecasting system must be able to produce calibrated uncertainty sets for its forecasts*. A consequence of this observation, before even stating the need for AI to produce uncertainty distributions and not just point estimates, is that the loss functions will typically be much more expensive to compute between prediction and data, typically having an n^2 computational complexity flavor [13]. New loss functions that are scalable for distribution prediction are needed.

Following are descriptions of several other classes of methods that are required from foundation models.

Quantifying the characteristics of clean energy resources through advanced forecasting techniques for wind, solar, and precipitation, which are pivotal for planning and development, is crucial. Such forecasting is also critical for inverse design system optimization. Operational (minutes-hours-day ahead), site-specific, and high-resolution resource forecasting for predictive dispatch control of clean energy generation and variable load resources are also needed to achieve system load balance and dynamic stability.

Equally important is improving load prediction accuracy, especially during extreme weather events, where behaviors of consumers in fulfilling essential needs — such as the increased use of air-conditioning during a heatwave — must be anticipated. This need can be described as forecasting and state estimation for better look-ahead loads and variable generation with (1) improved state estimation and prediction of grid conditions, and (2) outlook for anomalies that could impact operations.

Methods that more accurately forecast demand increases prompted by technology adoption and policy regulations are also needed. This encompasses decarbonization efforts, such as the retrofit of buildings for energy efficiency, and the increasing electrification of transportation, building, and other industry sectors. Accurate forecasts at the transformer and substation levels are critical for informed decision-making regarding the necessary upgrades to distribution systems.

We also identify the development of methods that establish and update improved default designs to meet regulation and performance requirements as a key needed advancement. Such methods will enable a more efficient response to issues raised during design and project reviews, both internally and externally.

Additionally, prediction of demand flexibility from building loads, EV charging, and the utilization of distributed energy resources (DERs), such as photovoltaics and storage, requires consideration of customer behavior, grid pricing signals, incentives, and local weather conditions, as well as the advancements and adoption of technologies. Demand flexibility is recognized as a pivotal mechanism to mitigate peak grid demand and to facilitate cost-effective and emissions-reducing operations.

The adoption of continual learning methods that assist operator-in-the-loop systems is another need, using real operational data for the development, implementation, and operation of these systems, thus supporting operators more effectively.

Last, facilitating the review and approval processes of new renewable energy projects by learning from past projects and databases has been proposed. AI-based assistance could significantly expedite these processes, reducing both costs and the potential loss of opportunities. Multimodal LLMs trained on data from thousands of past environmental and permitting reviews could also be developed to improve and expedite those process, similar to the foundation models discussed for improving the nuclear regulatory process in Section 1.1.

Connections to Experiment, Simulation, and Theory

Sophisticated control methods are essential to managing both the generation of energy and its consumption within the grid, whether that is directly at the point of connection or across the integrated system. These require considering the dynamic coupling of base and dispatchable generation (nuclear, hydro, geothermal, hydrogen), variable generation (solar, wind, wave), variable load (fuel, ammonia, hydrogen, etc., production), and battery storage operated as a single integrated system for dispatchable generation through coupled AI systems. To accurately predict and optimize the performance of this integrated energy system, foundation model-scale surrogates are needed for modeling and simulation of aggregated renewable generation components (wind, solar, marine hydrokinetics) as a single generator system operating in complex (temporal and spatial) probabilistic resource environments. These models must account for the varying and unpredictable nature of renewable resources over time and space. At the plant level, adaptive, surrogate models based on real-time measurements are needed to enable rapid adjustments to the system controls, which is essential for managing the changing dynamics of energy supply and demand. This high-fidelity, system-level digital-twin model could facilitate continuous system performance assessment, including of power grids and urban load centers and operations based on data and feedback control. The following are additional needs and connections between experiment, simulation, and theory to support future U.S. power grid needs:

- AI design tools derived from high-fidelity modeling (HFM) numerical simulation and field operational data.
- AI replacement modules in HFM simulations to accelerate processing and replace lower-fidelity empirical formulations and look-up tables.
- Digital twin and surrogate models for performance monitoring, operations and maintenance (O&M), and coupled edge computing for active and closed-loop control.
- AI orchestration in multiple-scenario digital twins to run simultaneously.

NEW TYPES OF MODELS, TOOLS, OR WORKFLOWS

Leveraging foundation models for planning, operating, and securing the power grid of the future will depend on the development of new tools and workflows. Workflows need to be modernized to allow for providing AI assistance to operators in a semi-autonomous fashion for emergency control to manage critical functions like load shedding and islanding during outages. These systems must respond in real time to prevent widespread disruptions, and, given the high-consequence nature of this system, a trusted AI-assisted operator workflow must be part of the solution. Moreover, this workflow needs to facilitate faster identification and correction of faults. A component of this need is a unified communication framework linking control centers to distributed energy resources so that geographically and functionally distributed elements can effectively relay information, optimizing real-time responsiveness and coordination.

A tool that is critical to any use of AI for power grid planning, operations, or security is an explainable and trustworthy interpretable AI-enabled decision support system. This capability must also be coupled with robust tools for their verification and validation (V&V). Tools are needed that not only perform tasks but also provide insights into their decision-making processes, a capability that is crucial for sustaining trust and reliability.

SCALE OF TEAMS NEEDED TO HAVE CONFIDENCE OF SIGNIFICANT PROGRESS

Developing and operationalizing foundation models to support planning, operation, and security for the U.S. power grid — a complex and critical infrastructure — requires an interdisciplinary and well-coordinated effort. The scale and types of teams needed can be broken down into several key areas:

- *AI and Data Scientists (~100 professionals):* A team of AI and data scientists will be essential to developing, training, fine-tuning, and maintaining foundation models. These professionals should have expertise in machine learning and deep learning and in developing safe, secure, and trustworthy AI.
- *Power System Engineers and Analysts (~100 professionals)*: An equal number of electrical engineers and energy system analysts with domain knowledge will be crucial for framing problems in a way that AI can address them and having a deep understanding of the U.S. grid's intricacies. They provide insight into the operational, planning, and regulatory nuances of the power grid and will help guide and ensure that relevant transformational AI is developed and deployed.
- *Software Engineers and System Integrators (~200 professionals)***:** To ensure that foundation models are implemented effectively, skilled software engineers and system integrators are needed. They will be responsible for embedding AI models into existing infrastructure and helping to design grid infrastructure. These professionals must develop software and systems that are safe, secure, and trustworthy and, given the various grid management systems (existing and to be developed), this is a daunting task given the increasing complexity of edge devices and systems drawing load from the grid.
- *Cybersecurity Professionals (~100 professionals)*: Cybersecurity professionals must be involved to safeguard systems that incorporate AI against intrusion and tampering, ensuring the integrity and security of the grid, especially with the increasing reliance on automation and autonomy for operator assistance.

Making significant progress in developing and operationalizing foundation models for the U.S. power grid will depend on tightly integrated teams that bring together AI technical knowledge and domain-specific expertise. While the scale of these teams will vary depending on the size and scope of the solution, adopting a comprehensive approach involving these various skill sets is necessary to building confidence and accelerating momentum in the progress being made.

SCALE OF MODEL BUILDING, COMPUTING, AND STORAGE NEEDED

The power grid has been described as the most complicated machine ever built by humans. The system that was designed and built to run based on the physical characteristics of the connected devices is migrating to a system that runs based on the control code embedded in them and the software that orchestrates their operations. To give a sense of the state of the art today, the ExaSGD project has run HiOp on Frontier to solve for networks with 10,000 buses under thousands of contingencies on parallel machines equipped with both AMD and NVIDIA accelerators. This calculation included 32 renewable energy forecast scenarios and 1,000 contingencies and was run on 4,096 nodes of Frontier [14]. Advancing the development of new foundation models will require tens of thousands of GPUs and the ability to process a hundred or more petabytes of data. The data for training may be limited unless the workflows described earlier are implemented. This plan will enable the training of a foundation model on domain data (PMUs, edge data, network traffic, smart meters, and more) to plan, operate, secure, and manage grid assets including digital twins of the system that can churn through tens of thousands of potential scenarios and courses of action.

DEPLOYMENT OF MODELS AND APPLICATIONS

AI can only help in the design and operation of the power grid if explainable and trustworthy AI models and applications are built. In other words, the scenarios derived from those models and applications must comply with constraints and improve upon the confidence that other objectives will be met while maintaining resilience when faced with unexpected disruptions. Extensive evaluations will be required to verify the performance of models and application and thus to ensure operations that are fully secure and reliable.

CRITICAL PARTNERSHIPS

The National Oceanic and Atmospheric Administration (NOAA) and National Aeronautics and Space Administration (NASA) have some of the most crucial datasets available for the characterization of the atmospheric states, and most AI products are trained on reanalysis data that either agency provides. Enhancing the resolution of atmospheric forecasts and downscaling will greatly benefit from interaction with both agencies. Other critical partnerships include the utilities and system operators of the power grids and other energy infrastructure assets who have extensive data and information on their systems.

RISKS, SAFEGUARDS, AND SECURITY REQUIREMENTS

Integrating AI into power systems planning and operations can offer important benefits, such as improved efficiency, enhanced reliability, and greater resilience. However, it may also come with important risks and challenges, which need to be carefully and thoughtfully addressed. Energy infrastructure has the unique feature that, despite being physically connected, access to the various data sources is geographically and physically distributed — not least by ownership. Moreover, some of the data are defined by critical infrastructure regulation and some of its conclusions may be subject to security review or concerns. Among those concerns is preventing data access by malevolent actors while maintaining access among infrastructure partners. An important need is to consider AI that is logically coherent but physically distributed and for which the training data can be ensured to have differential privacy for the various providers.

WORKFORCE AND TRAINING REQUIREMENTS

Vast amounts of knowledge on how to plan, operate, and secure the power grid must be transferred to the next-generation workforce. Current workforce training programs do not take advantage of how AI can speed this learning and help system designers and planners manage a workforce that is experiencing rapid turnover. New training methods are needed to help current and future grid planners and operators become more cognizant of AI's benefits and how to use AI applications in their field.

2.4 Expected Outcomes

The benefits of transforming to a clean energy system will be accompanied by the challenges of added complexity, variability, low visibility, and decentralization of the electric power grid. Preserving affordability and improving reliability, resilience, and security in the face of these challenges will require new thinking and approaches that would not apply to the centralized system of even the recent past. Selecting the best approaches is too complex a problem to be solved by human thought alone because of the number of possible combinations and outcomes. AI tools are needed to identify and select approaches that address complexity in matching generation to the times and places of energy demand to achieve an equitable energy future.

Distributed generation and the ability to manage local demand sources will require AI to generate a rich set of signals that maximize responsiveness and fidelity to utility objectives of selecting the cleanest, most affordable mix of sources, while maintaining reliable delivery. The growing body of information at the distribution scale will enable AI to optimize the deployment of energy storage to facilitate decoupling the time of generation from the time of use. At the regional scale, AI tools will help support the expansion and management of transmission infrastructure to ease bottlenecks in getting power from areas of plentiful generation to areas of high demand. Securing a highly interconnected power grid against cyberattacks and making it resilient to all forms of disruption will require that AI be able to address the complexities and uncertainties more rapidly than malevolent actors can exploit them.

Power outages have a major economic and societal impact on the U.S. Additionally, an integrated system is fragile, leaving the system vulnerable to cyberattacks. AI-based tools can help improve the planning and design of the system to make it more robust, provide real-time detection and response to events, and assist with the detection of future vulnerabilities. For example, could AI have predicted the 2021 winter brownouts in Texas due to the cold, or could it have identified future supply chain issues like the availability of transformers that we are currently facing? Or could it have identified future vulnerabilities between infrastructure assets such as loss of water that halts generators, or a single road/bridge that must be crossed for repairs, or a main communication path that could be cut?

The careful, guided application of AI is the only option for tackling the complexity of such a large, interconnected system during such a profound transformation. AI will enable these improvements to occur much more rapidly, on timelines consistent with climate goals, while improving other important objectives such as equity and reliability. Simultaneously optimizing carbon emissions, reliability, equity, resilience, and affordability requires a level of sophistication, speed, and efficiency beyond current planning and balancing approaches.

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03. CARBON MANAGEMENT

Achieving America's goal of a net-zero carbon economy by 2050 will require developing an expansive new carbon management industry, one that can address mitigation of greenhouse gas (GHG) emissions, deployment and reuse of relevant infrastructure, and technical innovations that ensure safe and reliable implementation of these new solutions. These innovations must also be able to safely transport and securely store vast quantities of carbon dioxide (CO_2). The technology and infrastructure we need must be deployed at an unprecedented pace and scale both nationally and globally. Success in this undertaking is an essential part of obtaining a secure, clean energy supply while reducing the climate impacts that increasingly threaten the safety, health, food supply, and economic security of our nation.

To meet this GHG emissions mitigation goal by 2050, U.S. infrastructure for carbon capture and storage will require capabilities to accommodate at least 65 million tons of CO_2 per year [1] —roughly equivalent to the amount used by today's CO_2-enhanced oil recovery (EOR) industry, which took over 50 years to develop. By 2050, annual subsurface storage capacity to accommodate ~one billion tons of CO_2 will be required. Storing CO_2 at this scale is likely to require at least 1,000 capture facilities, a 21,000−25,000-km network of interstate CO_2 trunk pipelines, 85,000 km of spur pipelines to supply the trunklines, thousands of injection wells [1] and appropriate subsurface storage reservoirs to accommodate this need.

Simultaneously, carbon management solutions are required to offset increasing demand for clean energy solutions. Clean energy production to address growing demand and offset decreasing production from conventional fossil energy sources are necessary [2]. Clean energy includes renewable energy resources, but also encompasses alternative resources such as unconventional critical minerals [3], geothermal, hydrogen, and nuclear energy.

Developing the necessary innovations to accelerate commercial deployment of carbon management solutions within the next 20 years will require maximizing and expanding existing infrastructure, developing hundreds of new facilities, and discovering innovative and efficient approaches, including novel subsurface analysis tools, transport modes, materials, equipment, and systems. Artificial intelligence (AI) and machine learning (ML) are needed both to expedite development and optimize the performance of this critical infrastructure and its components. AI's ability to quickly analyze complex engineered and natural systems will be critical for developing comprehensive carbon management solutions. Specifically, AI holds the potential to accelerate progress in our understanding of foundational science to identify the most important processes that affect our carbon budget. AI's ability to ingest multiple data streams to refine forecasts is needed to accurately assess the capacity and long-term integrity of subsurface environments, surface and subsurface mineralization processes, and other potential carbon containment resources—and to enable a highly reliable transport network that efficiently connects carbon sources to sinks. As the transport and storage industry grows, AI advances in optimization can also potentially minimize the risks associated with early demonstration and deployment projects and reduce basin-scale impacts.

3.1 Grand Challenges

CHALLENGE 1: "DISCO$_2$VER"

Addressing the need for an AI-enabled digital planet twin to accelerate clean energy transitions and inform safe and enduring greenhouse gas mitigation approaches.

An adaptive and integrated virtualized digital twin, data + models, and an enabling computational infrastructure are all needed to support real-time, rapid, and multi-scale simulation and forecasting to accelerate the U.S.'s transition to a carbon-neutral economy, mitigation of greenhouse gas emissions, and optimized security and deployment of energy infrastructure (Figure 3-1).

These carbon management and energy infrastructure systems often coexist, now or in the future with changing demographics, with other complex natural and societal systems that current simulation approaches cannot model holistically. Demands placed on existing infrastructure and resources as global populations and human activities increase, compounded by climate threats and more intense weather events, continue to stress our ecosystems and are more frequently causing environmental and human health impacts. AI's capabilities to bridge spatial and temporal scales will be critical in tackling these complex systems.

Using AI to create an all-encompassing, evolving digital twin of the planet, researchers will seek to accurately capture the range of engineered, environmental, and social activities, dynamics, and interactions across the planet to support the visualization, predictive modeling, and development of holistic planning and resiliency strategies.

If aggregated together in work on this digital planet twin, teams of researchers and commercial and regulatory stakeholders will have a better opportunity to rapidly forecast, simulate, and assess these complex, multidimensional, and multidisciplinary systems as a representative unit.

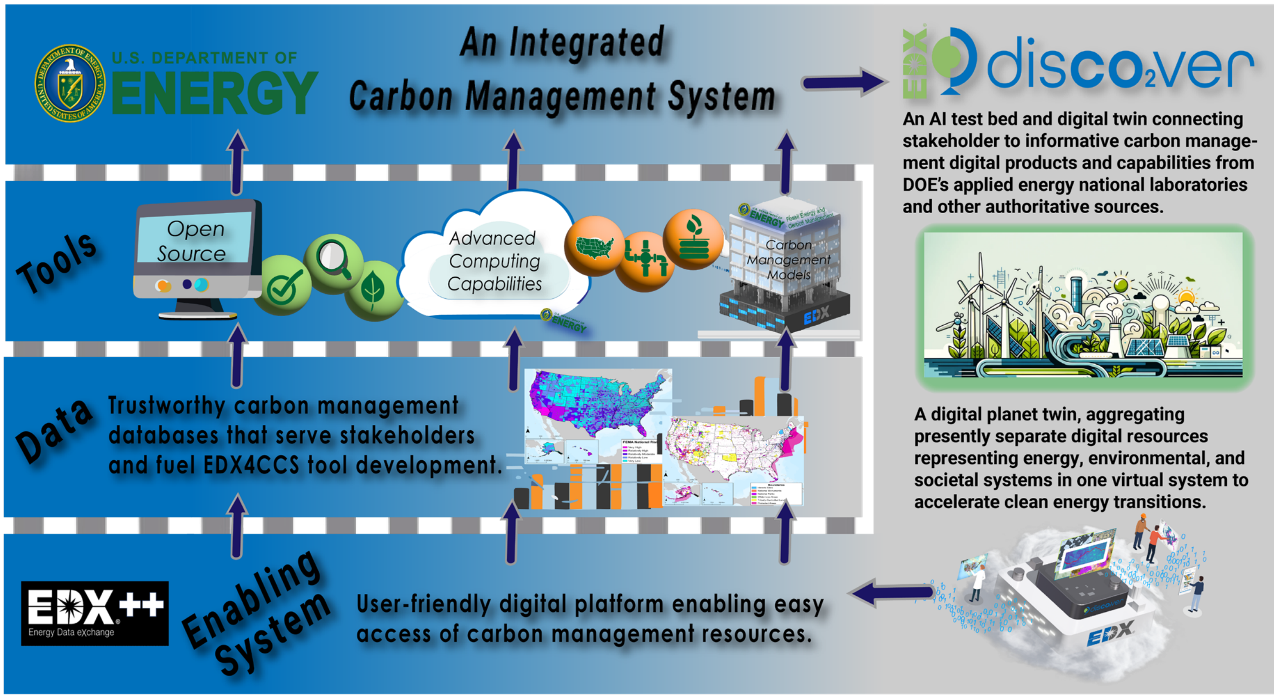

Figure 3-1. "disCO₂ver" would produce a digital planet twin, aggregating presently separate digital resources representing energy, environmental, and societal systems in one virtual system to accelerate clean energy transitions. (Image source: NETL)

Presently, where data, models, and tools exist to represent and/or analyze this complex system, they exist separately, leading to both a lack of understanding of the full coupled energy system or significant duplication of effort to find and utilize these resources, and also to the potential risk that vital data or tools will be missed by individual users.

While data and tools do not yet exist to create a complete digital planet twin, aggregation of what does exist — an authoritative integration — presents an opportunity to accelerate these goals and understand key gaps. Presently, existing science-based models and tools, (e.g., see some examples indexed on EDX disCO$_2$ver), data and knowledge resources for energy **sources** (e.g., solar, wind, geothermal, natural gas, coal, critical minerals, hydrogen, and nuclear), **emissions** (e.g., CO_2 and methane [CH_4]), **storage** (surface and subsurface), and **infrastructure** (orphan, aging, and emerging) present a significant opportunity to serve as the building blocks for a comprehensive model that accelerates carbon management, climate, commercial, and societal goals.

Individual science and sensing-based data and tools have been developed for systems such as the grid, CO_2 sequestration, geothermal, and individual infrastructure elements; but these systems have not been linked together for many reasons. First, even an individual system requires a high-fidelity model that often runs on high-performance computing (HPC). Second, the grand scale of a fully coupled model, a model of many joined models, currently requires significant computational resources and must be hosted in a virtual platform to support stakeholder benefits. Finally, systems typically fall within different funding agencies (e.g., Fossil Energy and Carbon Management [FECM], Nuclear Energy [NE], Energy Efficiency and Renewable Energy [EERE], Geothermal Technologies Office [GTO], U.S. Census Bureau, U.S. Department of the Interior, National Aeronautics and Space Administration [NASA], National Oceanic and Atmospheric Administration [NOAA], etc.) and have not been coupled together. Recent advances in **AI-based surrogate models in the cloud and using advanced computing systems (e.g., HPC)** have the potential to support development of an integrated data and multi-modeling coupled system, that is, a digital planet twin (Figure 3-1). Ultimately, such a digital planet twin would also support **AI-accelerated discoveries,** forecasting, and analyses such as:

- AI models that combine existing data and simulations (e.g., Earth systems, human behaviors).
- Utilization and repurposing of existing data to address new problems and keep computational costs low.
- Global AI models that can inform local problems for infrastructure planning, disaster mitigation, resiliency strategies, national security, and more.

Ultimately, this carbon management digital twin will support **disCO$_2$very** of solutions that support the administration of clean energy and emission mitigation goals by democratizing disparate models and resources to better represent complex Earth behaviors and thus help identify more strategic energy transition pathways that reflect current and forecasted communities, environments, climates, and infrastructure.

CHALLENGE 2: REALIZING A VIRTUAL SUBSURFACE EARTH MODEL

Making it possible to utilize the subsurface for environmentally friendly extraction of resources and safe storage of waste and emissions.

While complementary to the digital planet twin, the Earth's subsurface remains a significant, unknown frontier due to its opaqueness, remoteness, and heterogeneous nature. In order to accurately forecast subsurface energy resources and emissions, models require accurate input parameters which are difficult to obtain due to the challenge of interrogating the subsurface. While a digital twin of the planet's surface is viable with present knowledge and tools, exploration and prediction of subsurface properties and conditions poses a significant and complex but nevertheless addressable challenge.

By leveraging the data acquired over the past 150 years of subsurface exploration, in combination with science-based models and studies of the subsurface, we have a significant opportunity to leverage AI-informed methods to help identify and fill in the gaps about this important system that hosts natural resources and offers significant potential to store energy waste and products in support of carbon mitigation and clean energy transition.

The subsurface currently provides over 80% of our energy and over 50% of U.S. groundwater [4]. In the U.S., 4 million+ wellbores, resulting from drilling for hydrocarbons, now represent a treasure trove of direct and indirect information about the subsurface near each of these locations. The subsurface has potential to provide new, clean energy resources, such as geothermal, unconventional critical minerals, geologic hydrogen, etc. The subsurface also offers significant potential for the safe storage of resources (e.g., hydrogen [H_2], compressed air, etc.), while disposing of carbon waste (e.g., CO_2) [5] and other by-products (e.g., nuclear waste).

Current geophysical techniques to interrogate the subsurface result in a very incomplete picture due to limited spatial penetration of techniques and the noisy data that are collected. Recent advances in **AI for advanced property inference** show promise for utilizing noisy multi-modal data, along with science-based models of geologic and geophysical systems, to improve forecasting and prediction of subsurface properties and systems, informing and transforming our ability to utilize AI to virtualize subsurface systems, reduce risks, and interact responsibly with the subsurface (Figure 3-2).

Figure 3-2: Developing a more complete and assembled set of subsurface data, a virtual subsurface system, can help to inform, reduce risks, and drive better predictions using AI for aggregation of data and knowledge of the subsurface, and use of advanced property inference to fill in the gaps. (Image source: Gemini)

CHALLENGE 3: ACCELERATING IDENTIFICATION OF NEW MATERIALS AND/OR MATURATION OF EXISTING MATERIALS

Ensuring optimal performance and viability when deployed at commercial scales for carbon capture and removal.

Present materials for carbon capture face a scalability barrier, impeding their viability for large-scale commercial deployment. Using detailed, lab-scale materials data (e.g., solubility, permeability, surface area, isotherms, thermogravimetric analysis), AI could identify the key factors for optimizing critical functional properties that maximize carbon capture at scale while being economically feasible (see these reports for specific AI methods and opportunities in this arena).

In November 2021, Energy Secretary Jennifer Granholm announced the Carbon Negative Earthshot to remove gigatons of CO_2 directly from the atmosphere and durably store it for less than \$100 per ton of net CO_2-equivalent. This target calls for an all-hands-on-deck effort to innovate and scale up technologies in the growing field of carbon dioxide removal (CDR). The U.S. Department of Energy (DOE) defines CDR as a “wide array of approaches that capture CO_2 directly from the atmosphere [where CO_2 accounts for about 420 parts per million (ppm)] and durably store it in geological, biobased, and ocean reservoirs or in value-added products to create negative emissions.” The vast majority of climate and energy models for achieving net-zero emissions by 2050 indicate the need to develop and deploy these CDR technologies in the near term [6].

DOE research to support the Carbon Negative Earthshot explores diverse CDR approaches, including direct air capture (DAC), soil carbon sequestration, biomass carbon removal and storage (BiCRS), enhanced mineralization, ocean-based CDR, and other mechanisms. Fully investigating and understanding these approaches will help decision makers select the appropriate pathways to effectively meet U.S. goals and a range of community needs while achieving equity, cost, and sustainability targets [7].

AI for carbon capture and materials integrity discovery can help drive key technology breakthroughs and identify deployment strategies that are fit for purposes related to variations in geographic and operational requirements. This tailoring will be key to ensuring the viability of carbon capture deployments at commercial scales.

CHALLENGE 4: EMISSIONS PREDICTION, MEASUREMENT, AND MITIGATION

Addressing (1) hard-to-electrify sectors, heavy industry, and buildings, and (2) emerging threat(s) from unknown (passive, inert) sources (such as gaining energy infrastructure, wellbores, facilities).

Even with large-scale electrification, several hard-to-electrify sectors like rail, marine, and aviation and heavy industry like iron, steel, and cement production would continue to use liquid and gaseous fuels with potential for GHG emissions (e.g., [8]). Emissions arising from unknown sources such as infrastructure, historical resource, and legacy equipment need to be detected in a timely fashion for efficient abatement. Presently, there are technology gaps and other factors (e.g., aging infrastructure [9], weather events, etc.) that result in unintended and sometimes not immediately detected emissions (e.g., [10], [11]). Thus, a certain amount of GHG emissions are inevitable, while the rest could be stored or recycled. GC4 would feed into GC1 to develop clear criteria on acceptable levels of CO_2 emissions for these hard-to-electrify sectors and unknown sources. Individual tools to predict efficiency and emissions from these reacting flow systems exist for fossil-based fuels; however, they need to be adapted for low life-cycle carbon fuels (LLCFs) like H_2, methanol, ammonia [NH_3], and biofuels, etc. In addition, safe operation with these new fuels would require understanding and abatement of rare/catastrophic events like H_2 leakage, flame flashback, and blow-out, etc. The occurrence of low-probability but high-impact rare events poses critical challenges to performance and reliability.

There are risks of emissions, including of methane, CO_2, ozone, and more, from existing, aging, passive, and abandoned infrastructure. In the United States, natural gas and petroleum systems are the largest industrial source of methane emissions [12]. Other greenhouse gas emissions from industrial sources remain difficult to abate, while also accounting for trillions of tons of the CO_2 already emitted and present in Earth's atmosphere. Cumulatively, new and historical greenhouse gas emissions account for an estimated 10 gigatons of CO_2 ($GtCO_2$) globally that will need to be removed from the atmosphere annually by 2050, with up to 20 $GtCO_2$ being removed annually by 2100 [13].

Active industrial sources (e.g., steel, cement, and chemical manufacturing), along with orphan wells (documented and undocumented), abandoned pipelines, and storage facilities pose emissions and other risks to human health and the environment, now and as they age.

With land use changes, population changes, and climate change, the need to catalog, characterize, and forecast the future risks posed by these legacy elements will benefit from local to national-scale AI modeling. The opportunity exists for AI to assist with forecasting where these risks will emerge, particularly with changing climate and land use over time, as well as to predict what infrastructure is most susceptible to material degradation. AI will be enlisted to help model and discover alternative remediation technologies, such as wellbore plugging materials or approaches not yet viable commercially or technically or even discovered yet, or to help identify opportunities for alternative uses of some infrastructure to meet future needs while mitigating risks.

These cross-cutting problems are of interest across DOE offices such as FECM, EERE, Vehicle Technologies Office (VTO), Industrial Efficiency and Decarbonization (IEDO), and the Building Technologies Office (BTO), etc., and across other agencies like NASA, Federal Aviation Agency (FAA), U.S. Department of Agriculture (USDA), and others. Overall, GC4 aspires to improve system efficiencies by 30-40% (depending on the sector), which will result in subsequent reductions in emissions [5]. Recent advances in **AI and surrogate models, AI-based prediction, and control of complex engineered systems** will be leveraged to achieve this goal.

3.2 Advances in the Next Decade

CHALLENGE 1: "DISCO$_2$VER"

Addressing the need for an AI-enabled digital planet twin to accelerate clean energy transitions and inform safe and enduring greenhouse gas mitigation approaches.

Individual energy systems can provide detailed data sets that could be used to train large foundation models. Differential programming (e.g., AI for software engineering and programming) can be used to modify current science-based models of individual energy systems so that they are more effective within an AI model framework. Finally, a "mixture of expertise" model can be used to combine individual energy system models into a comprehensive coupled energy system model that can be used by planners and decision makers to perform scenario analyses of the coming energy transition(s).

CHALLENGE 2: REALIZING A VIRTUAL SUBSURFACE EARTH MODEL

Making it possible to utilize the subsurface for environmentally friendly extraction of resources and safe storage of waste and emissions.

High-resolution subsurface measurements under extreme conditions are now possible because of the rapid advancements in downhole characterization techniques, the advent of real-time geophysics, and new distributed sensing with fiber optics. These new methods produce big datasets that shift the data-scarcity paradigm, once very prevalent in subsurface science, to an emerging paradigm of multiple large yet noisy datasets that need to be combined and properly interpreted to better constrain subsurface simulation [4]. These geophysical techniques offer great potential but have economic limitations on their deployment and afford only indirect information about the subsurface. Reducing deployment and processing costs, as well as developing trustworthy validation approaches using science-based models and more sparse and directly measured data, will afford opportunities for AI-accelerated breakthroughs in improving the resolution and our understanding of the subsurface. **AI for advanced property inference** shows promise for combining these multi-modal data streams to especially key quantities of interest (e.g., the location of critical materials, permeability of formations, porosity, *in situ* temperature, pressure, and much more), thereby transforming our currently opaque view of the subsurface into a more transparent one.

CHALLENGE 3: ACCELERATING IDENTIFICATION OF NEW MATERIALS AND/OR MATURATION OF EXISTING MATERIALS

Ensuring optimal performance and viability when deployed at commercial scales for carbon capture and removal.

Emissions mitigation and materials strategies will require both point-of-source and direct air capture materials solutions. These include activities to build upon ***existing research on point source capture (PSC) materials to accelerate technology deployment*** [5] to capture far more concentrated CO_2 streams from power plants and industrial point sources than are viable to date. Large volumes of data on a range of materials and equipment are available (e.g., the National Carbon Capture Center) that can serve as information to drive breakthroughs in AI-informed PSC materials. AI modeling using this data and other resources for **material process data from PSC** could accelerate predictions and improve understanding of conditions, limitations, and process requirements of materials for DAC systems. AI may also help resolve how to **adapt PSC materials** (sorbents, solvents, etc.) for DAC applications. Designing energy-efficient systems for both PSC and DAC will also benefit from AI-based advanced optimization tools.

To resolve these needs for both PSC and DAC, science-based research and AI innovations are needed to:

- Improve material life and performance.
- Predict effectiveness of a material and process for specific site/boundary conditions.
- Predict impacts of impurities and atmospheric conditions.
- Predict better materials or make improvements to capture materials for commercial-scale operations.
- Predict and optimize materials and designs for electrochemical-based systems when they are significantly scaled up for commercial deployment.
- Predict costs of novel materials with scale up.

Other similar applications are discussed in more detail in DOE FECM's AI Needs in Critical Program Areas reports [14].

CHALLENGE 4: EMISSIONS PREDICTION, MEASUREMENT, AND MITIGATION

Addressing (1) hard-to-electrify sectors, heavy industry, and buildings, and (2) emerging threat(s) from unknown (passive, inert) sources (such as gaining energy infrastructure, wellbores, facilities).

Applied energy R&D is working to improve technologies to better detect, quantify, abate, and prevent methane emissions across the oil and gas supply chain [5]. This effort includes design of an Integrated Methane Monitoring Platform to continually collect, curate, and analyze data on thermogenic methane emissions. AI can transform emissions science because it can extract signal(s) from noisy datasets, thus reducing the threshold for detection and enabling more accurate quantification. AI can also be used to help decision makers with science-informed methane abatement and leakage prevention strategies. The platform's centralized software system and AI models will curate and analyze methane sensor data collected across various temporal frequencies, altitudes, and geographical ranges (local, basin, regional, and national scale) along with environmental data (wind speed and direction) to deliver accurate estimates of the sector's methane emissions. As AI tools and models in emissions mitigation are improved and validated, proven accurate, and earn industry confidence, they may inform the Pipeline and Hazardous Materials Safety Administration (PHMSA) process for developing new AGI codes and standards to mitigate and prevent methane leaks.

DOE-affiliated R&D programs are also supporting research, development, demonstration, and deployment (RDD&D) activities in methane mitigation [5] on undocumented/orphaned wells, pipeline integrity, geologic storage for hydrogen, and crosscutting issues. AI and ML [14] can assist in developing the capabilities to achieve these goals and help mitigate the most severe impacts of climate change.

In addition, the Exascale Computing Project (ECP) and other advanced computing resources (e.g., Cloud, HPC, edge computing) have delivered capabilities and tools that can be leveraged over the next decade to accelerate prediction of emissions from various energy systems to inform holistic and near-real-time understanding of sources, and how to mitigate these emissions. Foundational models can be generated from spatiotemporal evolution of the thermochemical state in flow systems, which can be utilized for prediction of normal and rare events. Rapid iterations in design processes are necessary with new LLCFs, which require the exploration of a large number of parameters, of which typically only a small subset of parameters have been historically modified. AI also offers capabilities for automated discovery and assessment of the underlying precursors and causalities governing rare events. Such capabilities are essential for the development of prognostic and control strategies to enable safe operation of these devices [15].

3.3 Accelerating Development

The resources needed to accelerate carbon management solutions to meet 2050 goals are largely cross-cutting in nature. DOE FECM has evaluated and documented AI R&D opportunities for accelerating the needs of the four key carbon management challenges above [14]. Thematically, all four challenges align to specific areas that can be addressed to accelerate a safe, secure, and AI-informed clean energy transition. These include:

- Data Aggregation: Many large data sets exist, but they need to be aggregated to enable AI training. A central repository that unifies the geoscience, applied materials, social, environmental, and other data resources that align to carbon management systems will help accelerate the research priorities described above, as well as highlight gaps that can be mitigated with new collection or synthetic data acquisition efforts. In the applied energy space, the Energy Data eXchange® from the National Energy Technology Laboratory (NETL)/FECM and several program-aligned renewable energy data hub platforms hosted by the National Renewable Energy Laboratory (NREL) offer more than a decade's worth of resources upon which this effort can continue to build.
- Data Veracity: We will need to further leverage ECP codes to develop gold-standard datasets for the full energy system. As necessary, high-fidelity experimental datasets would also need to be generated to validate the models. Curation of multi-modal scientific data sets, fusing experimental and computational data sets to develop surrogate models that can be used for robust design optimizations, would be essential.
- Methods: Transformer and next-generation ML architectures must be developed that can handle very large context windows beyond the 100k token windows that state-of-the-art large language models are using in order develop foundation models capable of accurately forecasting these complex coupled energy systems. Some work, as with Cross-attention and Mamba, has already started in this direction. Key breakthroughs are needed to reveal the underlying causalities associated with rare events, including advances in the following: deep generative models for representation learning, interpretability, and uncertainty quantification (UQ) in deep learning to reproduce and predict rare events and improve model robustness and trust; causal reasoning with AI to understand the root causes of rare events; asynchronous active learning approaches to tackle data imbalance; and scaling of AI methods to handle large simulation and experimental datasets. Multi-scale sequence modeling architectures are also needed that can scale to diverse multi-modal and multi-resolution data sets.
- Workflows: Current physics-based models will need to be modified with techniques such as differential programing to make them compatible with AI workflows. These workflows will need to couple disparate energy system models into a comprehensive digital twin of the full energy system.
- Connections to experiment, simulation, theory: Validating AI models is very different from validating traditional physics-based simulators. In order for these models to be trustworthy, both theory and experiment need to be carefully integrated into AI workflow to both constrain and validate these models.
- Test beds: The field needs to provide environments that support development of trustworthy, real-world applications of AI [16]. DOE's applied energy labs have several existing test beds developed for carbon management purposes, including (1) DOME (Demonstration and Operation of Microreactor Experiments), (2) LOTUS (Laboratory for Operations and Testing in the U.S.) Test Bed, (3) the Energy Data eXchange multi-cloud and advanced computing system EDX++, (4) EDXSpatial, (5) Cyber range, and (6) the ARIES platform.
- Scale of team: Diverse teams of experts with background in domain science, computational science, AI methods, workflow, and automation are necessary for success across the national lab system. Long-term (e.g., 5–10 year) investments are needed with a large team (e.g., 20–40 people each spending ~50–100% of their time on this effort would contribute to a good chance of success).
- Scale of model: This is a big open question, but we estimate that a model with less than 100B parameters could be trained that would have a transformational impact

on carbon management. The goal is that these large foundation models will exhibit emergent properties such as “few shot learning” that enables these models to forecast a wide range of scenarios accurately without the need for a full retraining of the model.

- Deployment: We anticipate that this model could be deployed in a manner similar to how the Llama models were deployed. With <100B parameters, it should be possible to perform inference or fine-tune the model, with the model residing on relatively modest hardware Deployment involves not only providing these tools to industry but also training them for appropriate use.
- Critical partnerships: Data-holders are key partners, including the U.S. Geological Service (USGS) in general, as well as the Earth MRI program, NASA, and the U.S. Environmental Protection Agency (EPA). Industrial partners, such as original equipment manufacturers of different devices, could add significant value if they can be coaxed into sharing data and will be critical to success. Partnerships with companies in energy resources, transmission, and production, as well as the technology industries are essential for mitigating emissions.
- Risks, safeguards, and security requirements: The release of such a model has the potential to induce the analogs of gold rushes — people flocking to extract value from parts of the earth that were previously not recognized as valuable. Ethicists should be brought in to help roll out the data and models safely. There are also growing concerns related to trustworthy data, both about its use to train AI models but also to validate and explain their outcomes. It will be crucial to ensure that data from the carbon management sector are robust and appropriate and fit for use — and that efforts are made to identify poor data or even fraudulent data before it is amplified in AI-informed applications for carbon management solutions.
- Workforce and training requirements: Acquiring a suitable workforce will be challenging given strong competition from industry. A robust DOE-wide training program for postdocs and staff would be valuable.

3.4 Expected Outcomes

CHALLENGE 1: “DISCO$_2$VER”

Addressing the need for an AI-enabled digital planet twin to accelerate clean energy transitions and inform safe and enduring greenhouse gas mitigation approaches.

Expected outcomes are to: (1) develop an accurate model to optimize different energy transition scenarios to maximize energy and minimize emissions; (2) minimize emissions of methane during production, processing, transportation, storage, and use across the coal, oil, and gas industry to eliminate nontrivial methane emissions from carbon-based fuel supply chains by 2030; and (3) advance cost-effective technology to identify, quantify, and predict methane leaks across sectors more efficiently and to improve both the accessibility and reliability of methane emissions data [5][14].

CHALLENGE 2: REALIZING A VIRTUAL SUBSURFACE EARTH MODEL

Making it possible to utilize the subsurface for environmentally friendly extraction of resources and safe storage of waste and emissions.

Expected outcomes are to transform our currently opaque view of the subsurface into a virtual system to inform and improve transparency both spatially and temporally so as to best utilize the subsurface for environmentally friendly resource utilization and waste storage.

CHALLENGE 3: ACCELERATING IDENTIFICATION OF NEW MATERIALS AND/OR MATURATION OF EXISTING MATERIALS

Ensuring optimal performance and viability when deployed at commercial scales for carbon capture and removal.

Expected outcomes are to reduce carbon dioxide to: (1) accelerate and enable optimal materials for commercial-scale operations; (2) ultimately, to help establish commercial viability of diverse CDR and PSC approaches in the service of facilitating gigaton-scale removal by 2050, emphasizing robust analysis of life cycle impacts of various CDR approaches and a deep commitment to environmental justice, including rigorously evaluating CDR, defining conditions for success, and leveraging leadership and expertise [5][14].

CHALLENGE 4: EMISSIONS PREDICTION, MEASUREMENT, AND MITIGATION

Addressing (1) hard-to-electrify sectors, heavy industry, and buildings, and (2) emerging threat(s) from unknown (passive, inert) sources (such as gaining energy infrastructure, wellbores, facilities).

Expected outcomes are to improve system efficiencies by 30–40% (depending on the sector), which will result in subsequent reductions in emissions. Traditional methods are not capable of delivering these advances in the next decade. Foundation models and AI-based surrogate models, together with leadership-class computing, will be indispensable to achieving the necessary emissions reductions in the next decade.

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04. ENERGY STORAGE

Independent of the technology used for energy production and effective distribution systems, energy storage will be a major component of future energy systems. Energy storage requirements at this magnitude demand a broad combination of different technologies to support the diverse needs of society, ranging from industry-scale, short-term buffers to stabilize the grid, to individual transportation modes emergency power backup, or seasonal storage for communities. The growth and demand for various energy storage systems meeting increasingly stringent performance requirements has become a primary challenge for the industry to adopt these technologies for various use cases. At the highest level, to meet the cost and performance targets, it is this extreme diversity of the solution space that makes developing new energy storage approaches especially challenging. At every stage, including material design, efforts to scale up, integrate, and operate multiple storage sites tied to the grid for various use cases are daunting and the most challenging tasks with current methodologies. We face an urgent need to dramatically reduce the development cycle from conception to deployment for energy storage technologies. The current processes take too long, and the complexities of managing the resulting storage ecosystem are too daunting to deliver solutions with the temporal and spatial coverage scales required to meaningfully address the climate crisis and maintain our competitive advantage.

4.1 Grand Challenges

We will first describe three grand challenges in detail and discuss how a strategic use of AI will enable disruptive advances that can massively accelerate development of the new storage technologies as well as the new paradigms that will reliably control and efficiently optimize the multi-scale storage networks within the next-generation power grid. Furthermore, for each grand challenge, the section will outline existing gaps and the critical research efforts necessary to realize the vision of ubiquitous and reliable energy storage.

CHALLENGE 1: RAPID DEVELOPMENT OF ENERGY STORAGE TECHNOLOGY

Given the need to decarbonize our energy systems and the growing demand for renewable energy, there is an immediate need to rapidly accelerate the development of affordable, high-efficiency, and secure energy storage solutions for the next generation. Global demand for energy storage is expected to grow by about 33% annually to reach 4,700 GWh by 2030, with revenue opportunities of over $400B [1]. The usual development cycle for energy storage technologies typically takes between 5 to 10 years. However, the current environmental and economic challenges require us to reduce the development cycle to mere months. This is a major challenge requiring advancements in materials discovery, scalable manufacturing, simulation technologies, product reliability, and cost effectiveness.

“A ten-times increase in the weight-oriented density of batteries would enable so many moonshots, if we can find a great idea. We just haven’t found one yet,” noted Astro Teller, Google X [2]. Transforming efficiency, reliability, and the resilience of energy storage technologies demands a deeper understanding and innovative strategies to manage the dynamics, which are determined by the underlying physical and chemical phenomena. Similarly, harnessing energy through heat storage holds promise for offering cost-effective solutions. Heat stands as the predominant energy form, constituting 50% of global final energy consumption. Currently, decarbonizing low-temperature heat (< 400°C) is relatively easier, while tackling high-temperature industrial sectors such as iron, steel, and cement proves to be significantly challenging. Strengthening our abilities in managing, storing, converting, and efficiently harnessing heat energy particularly within the temperature range of 400°C to 1500°C will be pivotal in preventing global warming from exceeding 2°C. Thermal energy storage and thermal transport stand out among the five thermal grand challenges identified in thermal science [3].

Designing energy storage systems is a prototypical example of a multi-scale and multi-physics problem, the solution of which may depend as much on understanding activation barriers, molecular-scale transport, thermodynamics, and reaction kinetics as it does on full-scale system design — and all scales in between. Each scale typically involves different computational tools, different experimental facilities, and most importantly, different types of technical expertise. As a result, designing, developing, and deploying a new storage solution involves many interdependent yet often isolated technical advances. Each of these steps may take years to mature, and failure in any one of them may reverse progress in all others. For example, a new material with great properties at the micro scale may later exhibit unwanted macro-scale behavior, prove corrosive or toxic, and degrade unexpectedly fast in a real-world deployment or prove incredibly hard to manufacture at scale. While some of these scientific challenges are unavoidable, one overarching technical problem is the slow transfer of knowledge and requirements between different aspects of the problem.

As with most other scientific disciplines, energy storage research relies on high-performance predictive simulations [4] to plan and analyze real-world experiments. However, even with the introduction of exascale computing, simulating an operational facility at atomistic fidelities is infeasible by many orders of magnitude. In fact, each scale of the problem typically employs its own approximations of the relevant physics, which may mean first-principles quantum dynamics simulations on one end and Reynolds-averaged Navier-Stokes solvers at the other. Within this ecosystem, each coarser-scale simulation model is fitted to match the finer-scale results to preserve the salient physics as best as possible. The challenge is that traditionally, both model design and fitting are laborious manual processes, and models are limited to a relatively small set of scalar inputs and outputs. As a result, it may take years for any breakthrough on the quantum scales to have any impact in prototype development, and more complex work cannot be accelerated easily. Instead, we need a new framework in which models at all scales are directly and automatically coupled and in which any expensive subcomponent can be replaced by a corresponding model. This shift in framework will enable a massive acceleration of high-fidelity models that easily and automatically integrate new developments and provide the predictive capabilities needed for rapid development and deployment of new storage technologies. We recognize that computational modeling approaches across such large spatial and temporal scales are intractable and need a new modeling paradigm to bridge the scales. In the past ten years, computational scientists have developed advanced simulation codes to expedite the discovery of energy storage materials through high-throughput screening and electrochemical transport analysis across different scales. Concurrently, experiments conducted at DOE science user facilities within multiple national laboratories have generated a significantly large quantity of data for investigating materials at nanoscale. Therefore, there is a unique opportunity for AI to fuse computational models and experimental data to enable a new energy storage materials development framework across traditional siloed scales [4].

The development of closed-form models with a relatively sparse set of input and output parameters both to ensure that the resulting approximations are scientifically valid and because existing statistical and modeling tools have been fundamentally restricted has been the limiting case. Notably, research from the last few decades on energy storage has created a plethora of data. For the existing energy storage technology, the time needed to analyze this data often exceeds the time it takes to collect it by a factor of ten. Moreover, when new manufacturing methods are needed for new materials, we need to adapt the existing models to the new systems.

Advancements in materials science are needed for accelerating the exploration of novel lithium compounds and solid-state electrolytes. These same developments can be extended to other technologies for the discovery of innovative thermal energy storage materials and synthesis methodologies for a wide range of operational temperatures, while satisfying all thermodynamic, kinetic, and functional property criteria. Specifically, energy storage technology needs new materials that can offer higher energy density, longer lifespans, natural abundance, and environmental friendliness. In addition, we need to innovate in scalable manufacturing technologies to automate and streamline production of energy storage materials. Such scalable technologies also need to be modular in the future so that they can be easily adapted to emerging demands and technological advancements. Automated quality control measures and rigorous testing protocols are required at every stage of the design and production to guarantee reliability and safety. Advanced data-driven monitoring and optimization technologies are needed to predict and prevent potential failures and to reduce material costs and improve efficiency. Finally, the incorporation of digital twins (DT) technology will become pivotal. For materials science, the challenge lies in developing computationally cheap but also accurate DTs to simulate and analyze many new materials before synthesis. DTs can significantly accelerate the discovery and testing of materials that offer higher energy density, longer lifespans, and environmental sustainability. In scalable manufacturing, the challenge is to develop DTs that can emulate the production processes. The virtual replicas of manufacturing systems enable automation and optimization and can offer promising methods to implement and evaluate rigorous testing protocols. These DTs can also be adapted for new and related systems. The overarching challenge is to cover the entire materials discovery workflow for energy storage through DT technologies with the goal of reducing the development cycle from decades to months.

CHALLENGE 2: EFFICIENT ENERGY STORAGE DEPLOYMENT, OPERATIONS, AND CONTROL

To completely decarbonize the electric grid and transition to net zero, we must address design, optimization, deployment, operations, and control of energy storage systems at the national level. Applications range from enhancing grid stability and resilience; to enabling decarbonization of buildings, transportation systems, and industrial systems; to realizing decarbonization of the power grid at large, given that energy storage at various timescales could mitigate intra-day and inter-season variability of demand.

Designing the location, type, and size of energy storage systems requires understanding the need for storage to support both mobile transportation systems, as well as stationary systems for the electric grid, buildings, and industrial processes.

Considering additional factors such as temporal/geospatial complexities, economic metrics (CAPEX and OPEX) and regulatory changes, etc., the optimal decision-making for energy storage systems siting requires evaluations of various scenarios that involve innumerable combinations of the aforementioned factors. This need presents a significant barrier to applying traditional approaches based on computationally expensive simulations, while presenting opportunities for generative AI or surrogate modeling approaches.

Real-time strategies in energy storage involve dynamic control and optimization of storage operations based on grid demand, renewable generation variability, and energy costs. Advanced predictive methods are required to forecast demand and generation patterns, enabling storage systems to charge during low demand or high renewable generation periods and discharge during peak demand. This real-time operational flexibility is crucial in managing grid fluctuations and ensuring a consistent energy supply. The need to respond to dispatch commands and maintain reliability is one of the major requirements for the flexible energy storage solution. Furthermore, we can enhance the reliability of a renewables-dominated grid by providing data-driven and proactive methods such as frequency regulation and voltage control.

Development of distributed energy storage systems is an important area for energy storage deployment. Distributed systems can enhance local grid resilience and provide communities with greater control over their energy sources. Such transformative deployment methods are critical for areas where grid stability is a major concern, such as remote or underserved regions in the country.

The distributed energy storage system should augment existing grid infrastructure to provide peak-shaving capabilities. The deployment of these distributed energy storage systems should be optimized to reduce the critical points and stresses in the grid and to mitigate supply-demand mismatches. One of the possible pathways is to aggregate the distributed energy resources as virtual power plants that can supply resilience and provide grid services like a traditional power plant [5]. To ensure a steady and reliable power supply, the distributed energy storage deployment strategy will need to manage the variability of stochastic energy resources such as wind and solar. In effect, we need a fully integrated smart grid, where energy storage technology will become one of the fundamental blocks of the grid architecture. This functionality may provide long-duration storage solutions to manage seasonal demand variability in energy generation and consumption. We must develop integrated solutions that holistically consider technological advancements and also the economic, regulatory, and social aspects of energy storage. These solutions should be scalable, adaptable to different geographic and socioeconomic settings, and should pave the way for an equitable energy transition. Additionally, understanding the lifecycle performance, material flow, and recycling aspects of energy storage technologies as they are developed, implemented, and managed will be crucial, as we aim for system circularity. Given these complexities, transformative and scalable solutions are required.

CHALLENGE 3: EQUITABLE AND ACCESSIBLE DEPLOYMENT

Equitable and accessible deployment of energy storage solutions is important to ensure that the advancements in energy storage are beneficial across diverse markets and communities.

Significant reductions in operational costs can be achieved through a wide range of energy storage system optimizations such as fast and efficient charging and discharging cycles and predictive maintenance. These cost reductions will be critical for extending the benefits and advantages of advanced energy storage solutions to a broader range of communities. In fact, significant barriers exist to achieving widespread, equitable deployment. For example, operational cost savings can be realized via optimizations in energy storage systems, such as through quick, efficient charge/discharge cycles and predictive upkeep, which are key to expanding the reach of sophisticated energy storage to more communities. However, some communities may have limited access to advanced technologies and connectivity. Overcoming this challenge is not trivial as it requires initiatives to enhance smart energy infrastructure in these areas. Moreover, it is crucial to ensure that the design, deployment, and control of these systems considers the diverse energy needs and economic constraints of different communities. To that end, we need to develop equitable solutions based on diverse settings that can reflect various socioeconomic, environmental conditions, and requirements. Furthermore, establishing supportive policy frameworks and partnerships are essential to deploying energy storage technologies in underserved regions. Strategic collaborations among technology developers, governments, not-for-profits, local utilities, and community leaders can facilitate an understanding of local needs and help customize energy storage solutions. Equitable and accessible deployment will help ensure that the benefits of renewable energy are distributed widely. Equitable and accessible deployment should also consider the workforce requirements for energy storage and how to prepare diverse communities to engage in the opportunities for this emerging technology.

4.2 Advances in the Next Decade

Prototyping and exploring different storage solutions will benefit from density functional theory (DFT) simulations enhanced by AI surrogate models for accurate predictions of material behavior under diverse conditions. Generative AI models will explore vast design spaces to identify optimal design configurations for energy storage solutions, taking into account various factors such as durability, efficiency, and cost. Deep reinforcement learning (DRL) will be used to automate the testing and optimization process, enabling the system to learn from each iteration and progressively improve the design. AI-enabled optimization and inverse design methods will be crucial for efficiently navigating the design space, balancing exploration with exploitation to quickly converge on the different storage solutions. Last, surrogate modeling will offer fast approximations of complex simulations, significantly speeding up the prototyping phase by predicting the outcomes of the computationally expensive experiments without the need for exhaustive testing.

Over the next decade, autonomous discovery in energy storage will leverage specific AI techniques to revolutionize material discovery and optimization. Generative models such as generative graph neural networks and generative language models trained on material data will be central to creating complex multimodal data representations, enabling the synthesis of new material structures by learning from existing datasets. A crucial element of effective machine learning atomic potentials is a robust descriptor or input vector that accurately captures molecular information that could be utilized by algorithms like neural networks to understand and forecast features such as bond dissociation energy or activation energy. As the generative models construct designs based on large datasets, a chemically consistent graph with stoichiometry constraints that allow for prediction of the most probable pathways to desired products in massive reaction networks could accelerate studies that have previously been impossible. Physics-Informed neural networks will ensure that AI models adhere to physical laws, enhancing the reliability of predictions for unseen materials and scenarios. Graph neural networks will be critical in capturing the complex interactions within materials at an atomic level, allowing for the efficient exploration of new battery materials and electrolyte solutions. Additionally, optimization and RL techniques will optimize the exploration of material space, guiding the discovery process toward promising candidates by learning from iterative evaluations and simulations.

In manufacturing, AI methods will include digital twin technologies that utilize deep learning algorithms for real-time monitoring and predictive maintenance, ensuring optimal production efficiency. Automated machine learning (ML) platforms will streamline the design of ML models for quality control, adapting to new manufacturing challenges without extensive human intervention. RL will optimize supply chain logistics and manufacturing processes, improving efficiency and reducing waste. For modular and flexible manufacturing systems, multi-agent systems will coordinate the actions of various components within the manufacturing line, enhancing adaptability and responsiveness to new product requirements. Predictive analytics will forecast production challenges and market demands, ensuring that manufacturing processes remain aligned with future energy storage needs.

Modern deep learning coupled with advanced computational workflows has the potential to solve the first challenge of rapid technology development by massively accelerating and improving predictive modeling at all scales. The key innovation is the ability of machine learning technologies such as generative models to ingest and produce a wide variety of data types as well as complex multimodal data. Consequently, any expensive subscale evaluation or phase in a multi-physics problem can be approximated using a neural network-based surrogate model. Conceptually, this statement holds true today, and surrogate models have been proposed to accelerate everything from chemical kinetics to plasma physics and from climate science to additive manufacturing. However, the accuracy of these models often remains questionable and, more importantly, existing solutions habitually fail to extrapolate to unseen situations. Consequently, simulations can be incredibly fast for known cases reflecting the training data, yet may fail to predict unobserved phenomena, which is one of their goals. Furthermore, no reliable uncertainty quantification or failure detection methods exist, meaning that problems often remain undetected and thus silently continue to provide incorrect results. Over the next decade, we expect these problems to be addressed through a variety of advances such as physics-informed models, multimodal foundation models, uncertainty and generalization theory, and automatic computational workflows.

Physics-informed models will inherently obey the known laws of physics and thus serve both to prevent nonsensical prediction as well as reduce the amount of data needed for training. Integrating multimodal foundation models will provide more reliable data representations for complex science data such as spectra, higher-order tensors, and the like. These have the potential to significantly improve the corresponding surrogate models by offloading the need to "understand" the data to the foundation model and reducing the surrogate to a simpler functional mapping in a convenient feature space. Finally, obtaining a better understanding of how confident a model may be in a given prediction and reliably detect prediction failures will enable an autonomous and nested multiscale modeling framework. For example, a coarse-level simulation may detect potential problems in a given surrogate via a high uncertainty score or a potential failure warning. This result can subsequently trigger additional simulation at the finer scales to re-train the given model and improve the solution. Automating and nesting this process will provide an ever-improving framework in which requirements for new information are passed to higher fidelities and the resulting improvements are directly integrated into lower fidelities.

AI can make a significant impact in accelerating materials science, specifically in the discovery and testing of new materials for energy storage such as advanced lithium compounds and solid-state electrolytes [6]. AI-based surrogate models can accelerate DFT simulations, which are quite expensive to run even on the largest supercomputers. For example, intrusive AI models can be used to replace the computationally expensive part of the simulation. Non-intrusive AI models can be used as surrogates for the simulation and experiments to predict the properties of new materials and narrow down the experimental space.

Significant early work on computational approaches to materials discovery can be traced back to the Materials Genome Initiative (MGI) (www.mgi.gov) [7]. The Materials Genome Initiative, launched in 2011, is a multi-agency initiative for discovering, manufacturing, and deploying advanced materials using machine learning and big data approaches to advance materials discovery. Among the big data approaches to materials discovery that grew out of MGI to further battery materials R&D is the Electrolyte Genome on battery electrodes and electrolyte materials. Computational approaches to rapid screening techniques seek to discover new battery materials and rapidly gain an understanding of electrochemical interactions and the development of physics-based performance models; these approaches are now at the forefront of battery R&D. A current example is the recently announced collaboration between Microsoft Corporation and Pacific Northwest National Lab (PNNL) on machine learning for advanced materials development. The team has reduced the computational materials development time from weeks or even months to days, and new solid-state electrolyte materials have been synthesized utilizing significantly less lithium than found in currently available batteries. This is but one example of the progress being made in early applications of AI to explore and identify new materials for advanced battery manufacturing in the U.S.

The U.S. Department of Energy's (DOE's) *Energy Storage Grand Challenge Roadmap* [8] outlines the national strategy to innovate, manufacture, and deploy energy storage technologies among various use cases [9], including by facilitating an evolving grid; serving remote communities; and pursuing electrified mobility, interdependent network infrastructure, critical services, and facility flexibility. The *Roadmap* proposes a policy and valuation framework, and it projects that the annual U.S. stationary energy market could grow from about $2 billion in 2020 to between $6 billion and $20 billion in 2030 [10]. In particular, the estimate of the global grid-scale battery storage market size was estimated to grow 24.4% annually from 2020 to 2027; and the deployment of 100 GW of energy storage by 2030 would create at least 200,000 jobs without accounting for a surge in U.S. technology innovation or expansion of domestic manufacturing. The national transportation decarbonization blueprint [11] projects that 50% of the new light-duty vehicle sales will be electric vehicles (EVs) by 2030, and the numbers for the medium- and heavy-duty EVs will be 30% and 100% by 2030 and 2040, respectively. In addition, the U.S. has lost $120 to $190 billion per year due to power outages and power quality degradation for all industries combined [12], which can be mitigated by the energy storage solutions. The resilience value of energy storage was further quantified by [13] depending on use cases: $10/kW-year for voltage support, roughly $100/kW-year for capacity and frequency regulation services [14], and $719/kilowatt-year for mitigating short-term outages.

A number of AI-based solutions have been proposed to manage the energy storage systems and thus achieve greater system and societal benefits. For instance, [15] summarizes existing reinforcement learning-based approaches to control and optimize battery storage solutions for various use cases (Figure 4-1). Deep Q-Learning-Based methods were proposed in [16] to operate the battery storage solutions considering the system uncertainties, while [17] aggregates electric vehicles as a power "battery" that participates in the energy and demand response markets using decentralized optimization techniques.

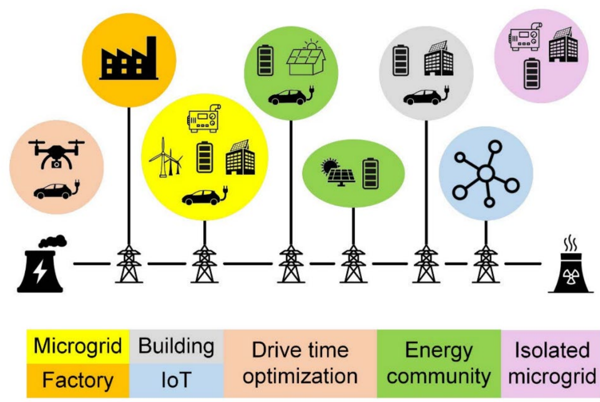

Figure 4-1. Application overview based on the review in [15].

AI tools and approaches can be used to optimize manufacturing processes for energy storage devices. The adoption of AI in automation technologies can improve production efficiency. From the initial design to the final assembly, AI has the potential to optimize every step of the various manufacturing processes. This optimization includes automating repetitive tasks and synthesis, optimizing supply chains, and controlling the quality. AI can also help in the development of flexible and modular manufacturing systems that are responsive to evolving technologies and market demands. Figure 4-2 summarizes examples of key opportunities and goals for AI to accelerate integrating historic knowledge with autonomous and automated experimentation and thus support R&D on energy storage.

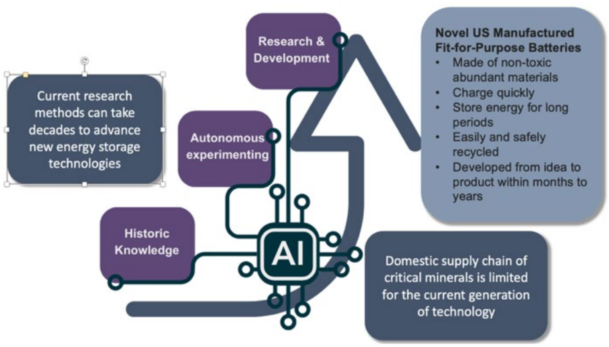

Figure 4-2. Opportunities and goals for AI to accelerate R&D for energy storage (Source: Ricarda Laasch, Lawrence Berkeley National Laboratory).

Proactive approaches to maintenance are required to ensure the long-term reliability and safety of energy storage technologies. To that end, AI can be used to implement advanced analytics to monitor, predict, and prevent potential failures in energy storage systems. The use of AI in developing digital twins can transform the way energy storage solutions are designed, tested, and maintained. AI-based DTs can provide virtual environments for rigorous, expansive, rapid, and inexpensive testing and optimization. These AI-based DTs can be adapted continuously to new simulation, experimental, and field data so that the testing environments are up to date.

Due to the variation in energy demand and the variability in renewable energy generation, we need a flexible and responsive control system for energy storage and by extension for the electric power grid. AI will reduce the complexity in managing the real-time operations of energy storage systems. AI, with its advanced predictive algorithms and models, can forecast energy demand and variable renewable energy generation patterns, which can be subsequently utilized to train more responsive and data-driven control strategies. This can allow energy storage systems to optimize the charge/discharge schedule. Furthermore, AI can optimize energy storage for frequency regulation and voltage control services, which are crucial for improving grid reliability. This AI-enabled, real-time operational efficiency will be key to managing grid fluctuations and ensuring a consistent energy supply.

AI can aid in the planning, design, and deployment of distributed energy storage systems. This is vital for enhancing grid resilience and for providing communities with control over their energy sources. Deployment optimization (driven by AI) will reduce the stressed areas of the grid and balance supply and demand. As we move toward more renewable energy, AI's role will expand to managing the variability of wind and solar power through these distributed energy storage systems.

AI-enabled grid infrastructure for the U.S. will advance our ability to manage energy distribution in a way that is affordable, efficient, reliable, and supportive of global decarbonization efforts. AI systems will be important for designing and operating a fully integrated smart grid, where energy storage is a fundamental component. AI can help manage long-duration storage solutions to accommodate daily, weekly, seasonal, and decadal variability in energy production and consumption. AI's role in this future grid extends to optimizing decarbonized grid planning and operation by minimizing energy losses and maximizing the use of renewable sources.

AI can enable energy storage solutions that are more adaptable and cost effective and can play a major role in democratizing access to clean and reliable energy. Tailoring energy storage solutions to the needs of different communities is one of the major benefits of a smart grid. AI can be used to analyze the different energy usage patterns, environmental conditions, and economic constraints of different communities. This effort will enable the holistic design and development of customized energy storage systems with different cost, efficiency, and reliability trade-offs. AI can make a significant impact in reducing the digital divide, one of the key barriers to equitable deployment of energy storage solutions. In many underserved communities, limited access to advanced technologies and connectivity hinders the adoption of modern energy solutions. AI, coupled with advancements in digital infrastructure, can help bridge this gap. AI can help us develop energy storage systems that are less reliant on high-end technological infrastructure or that can operate with limited connectivity.

4.3 Accelerating Development

Using AI to drive more rapid development of energy storage technology requires the integration of diverse and complex data types in the energy storage domain. This domain's inventory includes scientific papers, numerical simulation, experimental performance data, and environmental impact assessment data. AI can combine these data sets to accelerate materials discovery, improve designs, and predict long-term performance and environmental footprints. Having a common platform on which to collect and integrate such varied data is crucial for developing more efficient energy storage solutions.

Developing surrogate models represents a significant advancement in accelerating DFT simulations, a critical computational tool in materials science research. These surrogate models will be trained to approximate the output of DFT simulations and/or to replace the computationally expensive part of the simulation and thus enable fast predictions of the properties of new materials. These surrogate models learn to approximate the quantum mechanical calculations at a fraction of the time and computational cost.

The potential of multimodal AI foundation models in this context is significant. These advanced AI models are designed to process and learn from various types of data modalities. Development of foundation AI models will help us identify new patterns and correlations that are not feasible using traditional analysis methods. For instance, the generative AI models could generate novel material combinations for batteries by analyzing scientific literature and simulation data, predict the longevity and efficiency of these materials using real-world performance data, and assess their environmental impacts through environmental data. Once trained, the foundational models can be fine-tuned for various downstream tasks, such as predicting specific material behaviors under different environmental conditions or assessing new compounds for energy storage capabilities. This fine-tuning process involves adjusting the model parameters to serve the specific requirements of a task, which will improve the model's accuracy and applicability in diverse scenarios.

A diverse set of advanced AI methodologies is needed, including domain-aware, advanced foundational learning algorithms for handling complex multimodal data; transfer and few-shot learning tools for fine tuning and downstream predictive modeling tasks; tailored reinforcement learning and optimization methods; graph neural networks for modeling molecular structures; physics-informed AI methods for faster simulations; and interpretable and explainable and trustworthy AI for trustworthiness. Moreover, we need multimodal learning models, federated learning for privacy preservation and decentralized systems, and large language models for literature analysis and hypothesis generation.

The implementation of risk management strategies in AI-driven energy storage solutions is crucial for their safe, effective, and responsible deployment. These strategies need to focus on several key areas: alignment, robustness, uncertainty quantification, validation and verification, explainable and trustworthy AI, and security. Each of these areas plays a critical role in addressing the challenges of cybersecurity, bias mitigation, transparency, and resilience. With such trustworthy goals, we can minimize the risk of the AI system making decisions that are undesirable or harmful. This is particularly important in complex systems where AI might have to make trade-offs between different objectives. Robustness in AI systems refers to their ability to maintain performance under various conditions, including those that were not part of the training phase. This is critical in energy storage solutions where the system might face unpredictable scenarios. Rigorous testing protocols under various scenarios help ensure reliability and resilience. Uncertainty quantification involves assessing the reliability of the AI system's predictions and decisions. In the context of energy storage, it's important to understand the confidence level of AI predictions to manage energy resources effectively and to make informed decisions about energy distribution and storage. Validation and verification are crucial to ensuring that the AI system performs as intended. Validation checks whether the system meets the user's needs and requirements, whereas verification ensures that the system was built correctly. This element is essential in energy storage solutions to prevent errors that could lead to system failures or inefficiencies. The development of transparent and explainable and trustworthy AI models is key to addressing algorithmic biases. Explainable and trustworthy AI helps stakeholders understand how decisions are made, which is crucial for trust and accountability. Using diverse training datasets and regular assessments ensures fairness and effectiveness, reducing the risk of biased outcomes. Advanced cybersecurity measures are critical in protecting AI-driven energy storage systems from data breaches and cyber-attacks; this area includes authentication, encryption, data integrity, security audits, and intrusion detection systems.

The Integration of specialized wo"kflo's and tools is important for accelerating the development of energy storage technologies. AI-driven simulation platforms are essential for enabling rapid prototyping and testing, significantly reducing the time and resources required for developing new materials and products. These platforms leverage advanced AI algorithms to simulate and predict the properties of various materials and components, facilitating faster decision-making and iteration. The workflow integration plays a key role in enhancing overall efficiency. It involves the implementation of AI systems that seamlessly interconnect various stages of the development process, ranging from initial material selection to final product deployment. Workflow integration reduces bottlenecks and optimizes resource allocation by providing a smooth transition between these stages. This streamlined approach can ultimately contribute to faster adoption and scale-up of innovative energy storage solutions in the rapidly evolving landscape of renewable energy.

The diversity in expertise and perspectives expected within the various development teams, amounting to hundreds of professionals in total, will be critical to addressing the multifaceted challenges inherent in developing advanced energy storage solutions. Materials scientists are crucial for understanding the properties and behaviors of new materials and for guiding the AI algorithms in material selection and testing. Domain experts, including those with expertise in renewable energy, environmental science, and industrial processes, are vital for developing solutions that are not only technologically advanced but also viable, sustainable, and aligned with industry needs. The AI scientists will bring expertise in the advanced algorithms and machine learning techniques essential for analyzing complex datasets and refining AI models. Engineers play a pivotal role in applying the insights gained from AI and materials science to the practical design and manufacturing of energy storage systems.

The significance of high-performance computing, particularly through DOE leadership computing facilities and new AI supercomputers, is also critical. These advanced computing systems will be at the forefront of addressing the substantial computational demands required for training, enabling simulations that generate the training data, and deploying large AI foundation models. The integration of new AI supercomputers within these facilities marks a significant leap forward, providing even greater computational power and speed.

Ultimately, accelerating the deployment of AI models and applications in the field of energy storage hinges on integrating AI at the edge; developing smaller, fine-tuned models; guaranteeing model trustworthiness; and performing rigorous validation and verification. AI at the edge facilitates real-time data processing at or near the source, enhancing responsiveness and efficiency, both of which are particularly crucial for decentralized energy systems. Tailoring smaller, more specialized AI models from large foundation models for specific use cases ensures easier deployment and management, reducing the demand on computational resources. Trustworthiness, encompassing reliability, fairness, transparency, and ethics, is critical and is assured through thorough and rigorous validation and verification processes. Additionally, continual updates and improvements, driven by data and expert feedback, will be vital for maintaining the efficacy of these AI applications over time.

To this point, we have discussed the many ways that AI can be applied to accelerating the development and deployment of storage technologies in our energy infrastructure. One critical need to drive these developments is the generation of large datasets at all points in the development/deployment spectrum, facilitating adequate training of AI models and identification of key gaps. Current national laboratory-based projects have illustrated the promise of AI for energy storage, while also illuminating the limitations of having insufficient data to drive experiments. Thus, the need for data portends to be a key limiter in the development of AI for energy storage and must be capably and comprehensively addressed through active engagement in partnerships. DOE has identified this need and, through the Energy Storage Grand Challenge, has established a program called the Rapid Operational Validation Initiative (ROVI), which is designed to dramatically reduce the time required to bring new technologies to market. The ROVI effort is coordinated by six national labs and has already produced data requirements and guidelines for Li-Ion-based and flow battery-based systems [18]. Working with the Electric Power Research Institute, members of the ROVI team have published guidelines for data collection during monitoring of installed energy storage systems [19]. These types of efforts, coordinated through DOE leadership, help to standardize the collection of data from many experiments, installations, and partner organizations. In doing so, they provide the basis for accelerating AI applications that are described throughout the sections of this chapter.

Successful implementation of AI in this sector will depend on executing partnerships across academia, industry, and government agencies. Collaboration is necessary for sharing knowledge, resources, and best practices, as well as for aligning objectives and providing regulatory compliance.

The AI-driven transformation in energy storage technology will require a skilled workforce. Efforts to address this need span both the upskilling of the existing workforce and the recruitment and training of new talent with specialized AI skills. For the existing workforce, comprehensive training programs are essential to equipping it with the knowledge and skills required to effectively work with AI systems. These programs should cover a range of topics, from basic AI to more advanced algorithms, data analysis, and cybersecurity, and should be tailored to the specific needs of the energy storage sector. We also need to teach domain science to AI researchers. Recruitment strategies must also evolve to attract individuals who possess specialized AI skills. This talent pool will need to include computer scientists, applied mathematicians, AI model developers, and system integrators who can bridge the gap between AI technologies and energy storage applications. Universities and educational institutions play a crucial role by aligning curriculum with DOE and industry needs and by creating a new generation of professionals who are well-versed in AI and its applications in renewable energy. The pace of technological advancement in AI and energy storage means that skills and knowledge can quickly become outdated. Therefore, creating a culture of ongoing education and professional development will be essential to sustaining this ecosystem. This effort could involve regular training sessions, workshops, and collaboration with academic and research institutions to enable this future workforce to stay current with the latest developments and innovations.

To summarize, the advancement of energy storage technology with AI requires a comprehensive strategy that integrates varied and complex data sources that include scientific research, numerical simulations, experimental data, and environmental assessments. AI technologies need to implement domain-aware algorithms that can process multimodal data effectively, including surrogate models to speed up DFT simulations crucial in materials science. The potential of multimodal AI foundation models is significant, enabling the discovery of new patterns and the prediction of material'' properties, longevity, and environmental impacts. These AI models require task-specific fine-tuning that employ transfer and few-shot learning to improve predictive accuracy. Integrating physics-informed AI, graph neural networks, and interpretable AI will be vital to increasing simulation speeds and ensuring the trustworthiness of predictions. Federated learning and large language models can enhance privacy and literature analysis, respectively. Managing AI risks involves focusing on system robustness, uncertainty quantification, cybersecurity, and the necessity for AI systems to make reliable predictions under various conditions. New domain-aware validation and verification methods and the development of explainable and trustworthy and causal AI models will be critical for securing the trustworthiness of these systems.

4.4 Expected Outcomes

Leadership in Clean Technology and Market Growth: Focusing on domestic manufacturing technologies for scalable storage solutions will be crucial for achieving zero-emission goals by 2050. This effort aligns with global demands for sustainable energy storage, potentially unlocking a $10 trillion market. The development of more efficient and cost-effective storage solutions not only aids in meeting energy demands but also positions a nation as a leader in clean technology. This leadership can stimulate economic growth, create jobs, and foster innovation in the energy sector.

Operational Efficiency and Decarbonization: Improving storage operations to enhance cost-effectiveness and reliability directly impacts decarbonization efforts. Optimized siting/sizing, dispatch, lifespan prediction, and adoption of storage solutions by the grid and transportation sectors all serve to improve overall system efficiency. This advancement can lead to reduced carbon emissions and will support a transition to a zero-emissions economy. Furthermore, improving operational efficiency advances energy security.

Grid Reliability and National Security: Enhancing grid reliability will be vital to supporting the adoption of renewable energy sources and decarbonization. Bidirectional storage systems can accelerate the integration of variable renewable energy resources onto the electric grid. Reducing dependence on foreign materials and improving the supply chain for energy storage also strengthens national security. A reliable and secure grid is fundamental for economic development and national security.

Equitable Decarbonization: Addressing equitable decarbonization ensures that all communities benefit from the transition to cleaner energy sources. This approach involves considering the impact of energy storage and renewable energy (or lack thereof) on community health and resilience, especially in the face of extreme events and power outages. Additionally, creating a skilled workforce for energy storage technology development and deployment can lead to more equitable job opportunities and economic benefits.

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05. ENERGY MATERIALS

Energy materials play a key role in the generation, storage, and efficient use of energy and include, among others, materials for energy storage, photovoltaic and thermoelectric materials, catalysts, and advanced multicomponent alloys. These materials are key to designing solutions for efficient and renewable energy that will facilitate achieving U.S. goals in clean energy, economic growth, and energy justice while reducing dependency on non-renewable resources and minimizing environmental impacts.

Achieving U.S. sustainability and clean energy goals [1] by 2050 requires accelerating the discovery, design, production, and certification of energy materials with bespoke properties and performance. The discovery and design of new energy materials with specific properties and performance require the exploration of vast parameter spaces that are beyond the scope of human-driven exploration. In addition to understanding the fundamental properties of these materials, there are urgent needs to develop cost-effective and sustainable methods for their production and to address challenges related to their durability and lifecycle management.

Current developments in artificial intelligence (AI) play a multi-faceted role in advancing energy materials research by:

- Accelerating the design and discovery of new energy materials.
- Advancing laboratory automation to speed up synthesis, iterative testing, and refinement.
- Bridging the gap from laboratory-scale research to certified industrial-scale use.

Overall, AI has the potential to be a game-changer in the field of energy materials, able to uncover new materials, forecast their properties, and lead to discoveries that could address significant challenges in the energy sector. If we are successful, we will establish U.S. leadership in the development of high-performance but safe and clean-by-design energy materials that will accelerate the shift of the Nation toward a circular economy based on the sustainable and environmentally friendly reuse and regeneration of materials.

This chapter provides an overview of the most pressing challenges in energy materials and the new opportunities that the application of AI brings to advancing the discovery, synthesis, and scale-up of the production and use of a new generation of clean and safe-by-design energy materials.

5.1 Grand Challenges

Recent advances in AI have the potential to transform and accelerate the discovery and production of energy materials. Focusing on their applications, the most pressing needs in energy materials can be summarized across three main impact areas:

- **Energy generation, harvesting, and conversion.** Developing materials that enhance the efficiency and cost effectiveness of generating energy from renewable and nuclear sources is a priority. This objective includes improvements in solar energy technologies for better sunlight capture and conversion, advancements in extreme environment materials and fuels for safer and more efficient nuclear reactors, innovations in materials for hydrogen production, and development of thermoelectric materials to convert waste heat into electricity.
- **Energy storage and efficiency.** There is also a need to design materials that can store and convert energy more efficiently. This pursuit includes new materials for advanced batteries and supercapacitors that can provide better energy storage as well as improvements in fuel cell technologies and efficient hydrogen storage. Also needed are materials that can contribute to reducing overall energy consumption across systems, for instance, better insulation materials that are key for energy efficient buildings. Similarly, lightweight materials are required that enable energy conservation and efficiency across the transportation sector.
- **Environmental sustainability and scalability.** Another essential initiative involves reducing the environmental impacts of energy use and production. This requires the development of new materials for carbon capture and utilization that, by reducing atmospheric carbon dioxide (CO_2) levels, can contribute to mitigating climate change. It also includes the discovery of new catalysts that enhance the efficiency of energy-related chemical conversions, such as biofuels production. All future energy materials need to be designed to be sustainable and scalable for widespread use and mass production.

To address the above needs, the scientific community must focus on new scientific and technological advances aimed at:

- **Accelerating materials discovery** to identify novel material structures and compositions that can meet the functional requirements of different energy-related applications.

- **Improving predictive material design** to speed up the prototyping process and enable the efficient exploration of extensive variations across chemistries, transcending the current Edisonian (i.e., trial-and-error) approach.
- **Bridging the scales from lab experiments to industrial production** to enable rapid deployment and use of new materials.

The outcomes of such advances have the potential to enable new discoveries and technologies in energy materials that will be key in realizing further efforts to:

- Address the need for materials that support hydrogen production and CO_2 mitigation, alongside reducing dependency on critical materials like rare earth elements and lithium through the discovery of viable alternatives.
- Develop advanced fuel cells to reduce dependence on fossil fuels and support clean energy generation and a zero-carbon lifestyle.
- Speed up the qualification for new materials and nuclear fuels, especially those required for clean energy infrastructure and operation in extreme environments such as next-generation nuclear reactors.
- Design bespoke materials and parts for clean energy applications and infrastructure, such as solid-state transformers and structural materials for harsh environments like nuclear reactors.
- Discover new catalysts to generate “green ammonia” and accelerate deep decarbonization in agriculture through its dual use as a fertilizer and energy storage mechanism.
- Accelerate predictive design to speed up the prototyping process and explore extensive variations of material structures and compositions.
- Discover new materials to create high-energy-density batteries to improve the U.S. energy grid’s efficiency and resilience.
- Advance technologies for efficient CO_2 capture, storage, and transformation into high-value chemicals.
- Focus on unique applications in advanced manufacturing methods to create new, agile, and optimized supply chains.
- Achieve cost effectiveness and reliability in materials design to develop solid-state transformers that can replace traditional wire-wrapped systems.
- Accelerate the design process for energy materials, with an emphasis on predictive and inverse design to enhance energy efficiency.

The use of modern AI techniques can contribute to accelerating the development of new energy materials beyond what is currently possible if relying only on human interventions. However, significant scientific and technological challenges exist when applying AI techniques to energy materials research, including these:

- The need for vast datasets for AI/machine learning (ML) material informatics due to the heterogeneity of materials, which requires large investment and is time-consuming given that materials discovery and design must explore a potentially infinite parameter space.
- A disconnect between the current approach to materials science and the evolving pace of AI technology, necessitating a focus on ways to accelerate and increase efficiency, especially in upscaling from the laboratory to real industrial production environments.
- The need to overcome barriers such as the lack of rapid prototyping and achieving AI-driven advanced materials for bespoke energy applications that can support agile supply chains.
- The need to bridge the gap in scales in materials design, requiring AI to interpolate successive models and simulations, integrate experimental datasets, optimize multimodal functionalities, and address the disconnect in accuracy across temporal and spatial scales.
- The enormous computational costs associated with accelerating first-principles materials modeling, such as density functional theory (DFT) and other even more accurate and expensive methods, for generating the explainable and trustworthy AI models that are needed to predict material behavior with high fidelity.
- The need to identify the ways in which AI can play a role in meeting the grand challenges of energy materials by unravelling the process-microstructure-property relationships to optimize the process parameters for rapid and precise materials design.

The urgent need for better integration between materials science and AI will require both technological breakthroughs and new methodological approaches to drive advances in energy materials. We have identified three main challenges at the intersection of materials science and AI that that need to be addressed to transform materials discovery, synthesis, and manufacturing through a new generation of accelerated techniques for precision energy materials.

CHALLENGE 1: UNVEILING THE CAUSAL STRUCTURE OF THE ENERGY MATERIALS SPACE

Current materials data generation efforts such as the Materials Genome Initiative [2], combined with existing data on energy materials generated by U.S. Department of Energy (DOE)-funded projects (e.g., energy materials network [3], legacy irradiated materials performance database) and with experimental and computational data available across national and international repositories (e.g., Materials Project [4], Opencatalyst [5], NOMAD [6]), have the potential to enable rapid exploration of the energy materials space to accelerate discovery and design.

However, given the heterogeneous nature of these data and the distributed nature of the data resources, there is a need for a data curation and integration effort aimed at developing a latent representation of the energy materials space that includes materials structure, properties, performance, and lifecycle information. Creating and maintaining this latent representation require a continued large-scale effort to integrate existing and new experimental and computational data across modalities, scales, and fidelity levels. Such an effort will enable AI tools to learn a representation suitable to capturing and reproducing the causal structure of the multidimensional energy materials space. Modern AI techniques facilitate coupling latent space representations with large language models (LLMs) to provide the necessary alignment with materials science principles, as well as to facilitate the interpretability and explainability of potential paths across the materials space. These are key capabilities for guiding accurate and reliable inverse materials design. We anticipate that the generative capabilities of the latent space model will provide a new framework that can serve as the core of a future DOE-wide capability for science-informed autonomous discovery and design of new energy materials with targeted properties and performance.

CHALLENGE 2: ENABLING PRECISION SYNTHESIS AND MANUFACTURING OF ENERGY MATERIALS THROUGH REAL-TIME AI

The discovery and design of novel energy materials must be coupled to realizable synthesis processes. Modern AI techniques provide the appropriate framework for developing the next generation of AI-enabled synthesis and manufacturing platforms that can rapidly validate new synthesis routes and scale up to production using autonomous experimentation (AE) approaches. These platforms should range from single instruments with varied levels of autonomy to integrated, multi-instrument, self-driving laboratories (SDLs) capable of executing synthesis and characterization workflows with minimal human intervention. Precision synthesis requires the development of new AI capabilities that can leverage first-principles simulations to operate safely in regions of the materials space where limited data are available (i.e., extrapolation). There is also a need to codevelop artificial intelligence algorithms, heterogeneous computing systems, and real-time decision and control methodologies in concert with synthesis and characterization platforms to enable precision material synthesis [7]. In situ processing will require a new generation of edge-deployable AI models to steer the synthesis process in real time and achieve the precision needed to develop energy materials with bespoke performance. To help ensure the successful transition to industrial manufacturing, AI systems must be coupled to multiscale, physics-based simulations to develop industrial-scale digital twins that will inform the precision energy materials loop.

CHALLENGE 3: ADVANCING BEYOND MATERIAL PROPERTIES AND PERFORMANCE TO ACHIEVE LIFECYCLE-AWARE MATERIALS DESIGN

By leveraging advances in AI, the U.S. can accelerate the shift to a circular economy by incorporating the energy materials lifecycle into the precision energy materials loop. AI models need to be expanded to embed lifecycle and supply chain constraints into the materials design process to enable end-of-life recycling/upcycling and to minimize supply chain dependencies. Meeting these directives or constraints will require embracing new manufacturing methods and applying AI to generate ideas, anticipate how new materials will be used, and transition from rapid prototyping to testing and validation across various lifecycle stages. Achieving this goal will require the integration of AI-driven models for energy materials lifecycle with LLMs, fine-tuned with supply chain information, to support the decision process needed to optimize the design and production of high-performance but clean and safe-by-design energy materials.

5.2 Advances in the Next Decade

In the next decade, we anticipate a transformative change, driven by AI, in the way we discover, design, and manufacture energy materials. In this section, we will focus on the three areas where advances in AI will be critical to achieving broader scientific and technological impacts.

ACCELERATING ENERGY MATERIALS DISCOVERY

The field needs more refined techniques that enable AI tools to explore large chemical and materials spaces, screen and predict materials, discover feasible synthetic routes, and optimize multimodal functionalities using large datasets. Efficient and scalable methods to acquire high-quality experimental data and high-throughput computational simulations will be essential to building a high-fidelity representation of the materials space [8]. These advances should include efficient and reliable methods for extracting scientific knowledge from peer-reviewed literature, and new multimodal embedding techniques that capture and preserve existing structure-property-performance relationships in materials data. Advances in topological data analysis can provide new insights on the structure and properties of the high-dimensional data manifolds that represent the energy materials space. Progress in causal inference algorithms will also be needed to understand the underlying causal mechanisms in materials science. This includes the development of novel AI techniques to infer causal relationships from multiple data modalities. To accelerate discovery, researchers need to develop accurate AI-driven surrogates for computationally expensive first-principles simulations (e.g., electronic structure, molecular dynamics, phase field modeling) allowing more efficient navigation and selection of high-fidelity simulations across scales. Efficient data assimilation techniques must be developed that facilitate the continuous updating of the latent space representation as more data become available.

IMPROVING PREDICTIVE MODELING AND DESIGN

AI will be a significant player in accelerating the design process and predicting the properties of materials, thus reducing the time required for prototyping, development, and certification. AI capabilities that bridge the scales gap in materials design are needed, to interpolate successive models and simulations, integrate datasets, optimize multimodal functionalities, and attend to the accuracy discrepancies across different materials scales. Through advances in AI and multi-fidelity modeling, we will be able to predict and model material behaviors with high accuracy by connecting multiple data modalities, spatiotemporal scales, and physics. Applications of AI-enabled predictive models could range from predicting the microstructure of a material based on specific manufacturing parameters to forecasting material properties in extreme environments [9]. Advances in inverse design and reinforcement learning will be key in predictive modeling tasks exploring design space, synthesizing materials, optimizing multimodal functionalities, and designing bespoke parts for unique applications in the energy sector. Similarly, significant advances will be required to achieve explainable and trustworthy AI models that will facilitate the shift from high-throughput trial and error to precision materials by design.

BRIDGING THE SCALE FROM LAB EXPERIMENTS TO INDUSTRIAL PRODUCTION

Efforts are needed to enhance AI capabilities to accurately predict material properties and performance across scales to expedite the transition from lab-scale experiments to industrial manufacturing. Explainable and trustworthy AI models with reliable extrapolation capabilities will be needed to streamline the scale-up from laboratory to industry. Also, AI systems will need to be more effectively integrated with advancements in manufacturing technology. This effort should include real-time monitoring and adaptive control mechanisms that allow AI to respond dynamically to changes in the manufacturing process. Such a capability will require advanced AI techniques to facilitate real-time feedback for experiments and make crucial decisions during the upscale process.

Significant advances will also be needed in cross-cutting areas. For instance, in the DOE context, there is a need to integrate the unique instruments at the experimental user facilities and national laboratories with the leadership computing resources. Advancing in this direction, DOE's Integrated Research Infrastructure (IRI) [10] aims at facilitating this seamless integration through the future High Performance Data Facility (HPDF). The facility will provide the basic interoperability and governance mechanisms needed for data-compute integration and for the development of advanced AI solutions for materials science. There is also a need to ensure the sustainability of the software and AI-based models for energy materials. The uniqueness in the AI model development and validation lifecycle requires novel and effective provenance tracking. An additional complexity is the difference in resources and utilization workflows during model training or during inference. While DOE computing resources can provide a suitable framework for model training, the deployment of these models in production environments (i.e., close to the instruments) requires new approaches and infrastructure. For instance, advances in edge computing and hardware acceleration will be needed to facilitate model inference in latency-constrained environments. Advances in AI safety and trustworthiness will also be a crosscutting need when AI models will be integrated with synthesis and characterization platforms. The applied nature of the energy materials space will require developing new approaches to balance between sharing data for faster advancement and maintaining necessary controls for proprietary or sensitive information. Expanding on federated learning approaches and AI safety will be critical to ensure that proprietary data are not disclosed.

5.3 Accelerating Development

This section summarizes several areas where DOE needs to accelerate the development of resources to achieve our goal of accelerated precision synthesis and manufacturing of energy materials.

DATA AND KNOWLEDGE

High-quality data and mechanistic knowledge are key to developing and validating predictive models for materials. There is an urgent need to develop curated datasets that provide a diverse view of the energy materials landscape. This involves collecting, generating, and curating multimodal data that cover an extensive range of chemical structures, surface compositions, properties, and performance metrics across multiple spatiotemporal scales and operando conditions (e.g., irradiation effects). Efforts to develop new representations for energy materials beyond SMILES [11] or SELFIES [12] should be a priority. To enable predictive materials science, traditional approaches to data management need to be enhanced to support automatic metadata annotation and robust provenance tracking. The emerging properties of LLMs provide novel and effective approaches for knowledge extraction from data. Incipient efforts on using LLMs for materials data need to be supported and expanded. Reliable experimental data, either for model training or validation, are vital. Optimal experiment design techniques (e.g., Bayesian optimization, active learning) together with reduced-order surrogate models and generative models will be critical to reduce the cost of large-scale data generation for AI training. Optimal design should be complemented by high-throughput experimentation capabilities with highly automated characterization and synthesis instruments to generate adequate and meaningful datasets. Collecting data from industrial manufacturing processes to understand materials lifecycle, unique applications, supply chain issues, and how materials behave at industrial scales will be invaluable to modeling the transition from laboratory-scale experiments to industrial production.

METHODS DEVELOPMENT

To accelerate the development of precision energy materials, there is a need to accelerate the development of new AI methods. One of the priority areas should be the exploration of methods that learn from limited data (e.g., expanding beyond few-shot-learning) while allowing reliable extrapolation outside the training regime. Efforts bridging first-principles simulations with physics-informed machine learning need to incorporate elements of causal reasoning to provide explainable and trustworthy and science-aligned AI systems. Advanced AI techniques to bridge gaps in materials design across different scales must be developed to facilitate the interpolation of successive models. Specifically, we need to develop more efficient methods to explore large materials design spaces, increasing by 4–7 orders of magnitude the number of atoms that we can currently simulate from first-principles calculations. Also, new approaches based on model-free reinforcement learning and AI systems with compositional generalization capabilities can be used to recombine known concepts to understand and adapt to novel situations. This capability will be particularly relevant in the context of energy materials design, where different compositions of materials could be created and analyzed.

SCALE OF MODELS

Leveraging model modularity and composability we can create novel hierarchical frameworks for energy materials modeling. At the top of the hierarchy, a human-computer interface (HCI) based on an LLM handles the planning of high-level scientific tasks expressed as abstract concepts and goals set by domain experts. For instance, a user might state, “we want a material that does (*a, b, c*) and the constraints are (*x, y, z*).” The middle layer integrates various domain-specific foundation models for design space exploration that can integrate existing modeling and simulation capabilities. At the bottom of the hierarchy, a set of adaptive control models for smart instruments, tailored for specific applications, executes the synthesis and characterization tasks under the specific constraints imposed by the user (e.g., limit the use of critical elements) while continually learning and adapting to changes in the process. In terms of composability, each model in the hierarchy should be conceived as an interchangeable module. It means that for different applications, specific domain-specific models can be swapped out as needed. This modularity also allows for general models to be refined for different domains, for instance, by fine-tuning according to the specific requirements of the application. Moreover, hierarchical models can work alongside other AI techniques to handle the transition from lab experiments to industrial scales.

Regarding the scale of the models, we anticipate that the LLM for energy materials will be on the order of 1 trillion parameters, whereas the set of domain-specific foundation models will be in the range of 250 to 750 billion parameters. The adaptive models for smart instruments will be smaller (~10 billion parameters), but the need for continuous learning will pose significant computational challenges. For larger models, it is worth noting that as the frequency of retraining foundation models lowers, the established models are expected to stabilize and stand effective for longer periods of time.

SCALE OF COMPUTING

Model training and inference will need to span across all scales of the continuum computing. Edge computing, including domain-specific hardware accelerators, will provide a suitable infrastructure for real-time AI systems directly connected to the instruments. Edge systems need to be able to accommodate multiple latency constraints (e.g., from microseconds to minutes) depending on the dynamics of the synthesis and manufacturing processes. Existing mid-range and large-scale high-performance computing (HPC) facilities will need to increase in size (i.e., number of accelerators) to accommodate the training of LLMs. Finally, elastic cloud computing resources (both on premise and public) can provide support for the deployment of models in production environments, facilitating their access to academic and industry partners. There is a need to orchestrate and co-schedule workflows across experimental and computational user facilities. This capability will enable the hybrid compute deployment of federated AI capabilities. The ongoing IRI effort provides an excellent starting point for the integration of data and compute resources needed for the successful application of AI to advance energy materials research.

Advances in energy-efficient computing will be critical for the development of large-scale AI systems. The energy demand of training increasingly large foundation models is not sustainable; and thus, more efficient algorithms, smaller models, and energy-efficient architectures should be explored.

PARTNERSHIPS AND WORKFORCE DEVELOPMENT

To be successful in this effort, the need exists to establish critical partnerships across different labs, industries, and universities envisioning them as decadal-scale relationships.

In addition, relevant stakeholders including regulatory bodies need to be engaged throughout the lifecycle-aware materials design process to ensure that their needs are met and that potential risks are managed effectively. Relevant industry partners include instrument manufacturers and companies providing relevant data. Engaging with industry will also provide a path for technology transfer and commercialization that will have direct impacts on U.S. competitiveness and economic growth. Specifically, partnerships with equipment and instrument vendors will be critical for the tighter integration of AI with synthesis and characterization required for self-driving laboratories.

There is also a need to articulate and leverage connections across various national laboratories, where each laboratory can provide invaluable expertise and resources and can collaborate on shared goals. Additionally, collaborations should extend beyond DOE to include facilities related to other sectors like U.S. Department of Defense (DoD) or the U.S. Department of Commerce (DoC). Interagency collaboration (e.g., National Science Foundation, DoD, National Institute of Standards and Technology [NIST]) will be necessary for establishing a leadership AI computing capability.

Partnerships with universities will be critical for workforce development. There is a growing need for developing a unique skillset in the workforce that integrates both AI and materials science competencies. Universities can contribute significantly by incorporating AI and materials science expertise into their curricula to prepare the future workforce and could aid in the development of pipeline programs. Multi-agency funding could be a strategy to support the workforce pipeline, upskilling existing staff, and workforce development programs.

RISKS, SAFEGUARDS, AND SECURITY

One of the main risks related to AI use in energy materials stems from the access to some of the industry-owned data. There is a need to develop effective safeguards to protect such information while still allowing users to leverage insights from a model without violating proprietary data agreements. Advancing methods to avoid data leakage from AI models should be a priority. Approaches such as privacy-preserving AI methods and efficient AI algorithms to learn from encrypted data can help secure the data used for training the models.

Securing proprietary data can pose significant technical challenges, particularly in partnerships across facilities or in the face of industry collaborations. There are tensions between the impetus for collaborators to share data to advance more quickly versus managing data to ensure confidentiality and/or export controls. Ensuring compliance with existing regulatory standards, such as the NIST's AI risk management framework, is of utmost importance to avoid potential pitfalls and breaches, while providing opportunities for using federated, privacy-preserving methods.

Verification and validation (V&V) of AI models is an area that needs urgent attention and increased research efforts. Contrary to well-established V&V processes in software, the validation of AI systems provides significant opportunities for research and development. A specific area, relevant for AI applications in energy materials, could be developing approaches for “scientific red teaming” to verify that the outcomes of the AI system do not violate science principles.

5.4 Expected Outcomes

The AI-accelerated discovery, synthesis, and manufacturing of precision energy materials has the potential to deliver impacts akin to precision medicine. The use of advanced AI techniques and tools will increase the explorable materials space by several orders of magnitude. This expansion will, in turn, result in a significant reduction in the time and cost associated with the discovery of new materials for energy applications (e.g., solar cells, batteries, fuel cells, catalysts, nuclear fuels and materials, etc.). This accelerated discovery can lead to more efficient and cost-effective energy solutions that will contribute to U.S. energy security by reducing our dependency on imported energy sources.

By achieving precision control in the materials synthesis and manufacturing process, we will create new and highly efficient materials with specific property profiles and performance. For instance, the precise control of structure and properties will facilitate the design of improved fuels and structural materials for the next generation of nuclear energy systems. This efficiency can contribute to reduce energy consumption and improve resource utilization, not only in the U.S. but globally.

By including clean and safe-by-design constraints in the design of new materials, we will be able to reduce their environmental impacts and enable better reuse and recycling.

Finally, embedding supply-chain constraints in the design of new energy materials will contribute to leveraging the use of abundant U.S. sources of materials to avoid reliance on critical materials.

Overall, the development of advanced AI systems coupled with physics-based simulations in conjunction with DOE's unique experimental and computational facilities will transform the discovery, design, synthesis, production, and certification of energy materials. Thus, this effort will contribute to establishing U.S. leadership in applied energy.

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APPENDIXES

AA. AGENDA

THURSDAY, DECEMBER 14, 2023

Building 240, Room 1501

8:30 a.m. **Registration and Coffee**

9:00 a.m. **Welcome and Introduction**

- *Claus Daniel, Associate Laboratory Director (Argonne)*

9:15 a.m. **DOE FASST: Overview**

- *Rick Stevens, Associate Laboratory Director (Argonne)*

10:00 a.m. **DOE Program Offices: Panel moderated by Kirsten Laurin-Kovitz (Argonne)**

- *Alice Caponiti, Deputy Assistant Secretary for Reactor Fleet and Advanced Reactor Deployment (NE)*
- *Tassos Golnas, Technology Manager, Photovoltaics (EERE)*
- *Thuc Hoang, Director of the Office of Advanced Simulation and Computing & Institutional Research and Development Programs (NNSA)*
- *Darren Mollot, Director for Artificial Intelligence and Special Projects (FECM)*
- *Ceren Susut-Bennett, Associate Director, Advanced Scientific Computing Research (SC)*

10:45 a.m. **Morning Break**

11:00 a.m. **Exemplar #1: Nuclear Energy**

- *Chris Ritter (INL)*

11:15 a.m. **Exemplar #2: Power Grid**

- *John Grosh (LLNL)*

11:30 a.m. **Exemplar #3: Carbon Management**

- *Hari Viswanathan (LANL)*

11:45 a.m. **Exemplar #4: Energy Storage**

- *Charlie Hanley (Sandia)*

12:00 p.m. **Exemplar #5: Energy Materials**

- *Ian Foster (Argonne)*

12:15 p.m. **Working Lunch and Charge for Afternoon Breakouts**

1:00 p.m. **Energy Breakouts: Afternoon Session in Buildings 241 and 242**

- **Breakout #1: Nuclear Energy**
  - Location: Building 241, D173
  - *Lead: Rick Vilim (Argonne)*
  - *Co-Lead: Ahmad Al Rashdan (INL)*
- **Breakout #2: Power Grid**
  - Location: Building 242, J108
  - *Lead: Court Corley (PNNL)*
  - *Co-lead: Ben Kroposki (NREL)*
- **Breakout #3: Carbon Management**
  - Location: Building 242, J208
  - *Lead: Kelly Rose (NETL)*
  - *Co-lead: Sibendu Som (Argonne)*
- **Breakout #4: Energy Storage**
  - Location: Building 241, A323-T
  - *Lead: Prasanna Balaprakash (ORNL)*
  - *Co-lead: Mary Ann Piette (LBNL)*

- **Breakout #5:** **Energy Materials**
  - Location: Building 241, B123
  - *Lead: Robert Rallo (PNNL)*
  - *Co-lead: Brian Van Essen (LLNL)*

2:00 p.m. **Afternoon Break: Building 241, Room D286**

4:00 p.m. **Afternoon Breakout Session: Report-out Summaries in Building 240**

- Breakout #1: Nuclear Energy
- Breakout #2: Power Grid
- Breakout #3: Carbon Management
- Breakout #4: Energy Storage
- Breakout #5: Energy Materials

5:00 p.m. **Day One Adjourn**

FRIDAY, DECEMBER 15, 2023

Building 240, Room 1501

8:30 a.m. **Registration and Coffee**

9:00 a.m. **Charges and Organization for the Morning Breakouts**

- *Rick Stevens, Associate Laboratory Director (Argonne)*

9:15 a.m. **Energy Breakouts: Morning Session in Buildings 241 and 242**

- **Breakout #1:** **Nuclear Energy**
  - *Location: Building 241, D173*
  - *Lead: Prashant Jain (ORNL)*
  - *Co-Lead: Andrew Siegel (Argonne)*

- **Breakout #2:** **Power Grid**
  - Location: Building 242, J108
  - *Lead: Court Corley (PNNL)*
  - *Co-lead: Ben Kroposki (NREL)*

- **Breakout #3:** **Carbon Management**
  - Location: Building 242, J208
  - *Lead: Kelly Rose (NETL)*
  - *Co-lead: Sibendu Som (Argonne)*

- **Breakout #4:** **Energy Storage**
  - Location: Building 241, A323-T
  - *Lead: Prasanna Balaprakash (ORNL)*
  - *Co-lead: Mary Ann Piette (LBNL)*

- **Breakout #5:** **Energy Materials**
  - Location: Building 241, B123
  - *Lead: Robert Rallo (PNNL)*
  - *Co-lead: Brian Van Essen (LLNL)*

12:00 p.m. **Working Lunch and Morning Session Report-outs in Building 240**

- Breakout #1: Nuclear Energy
- Breakout #2: Power Grid
- Breakout #3: Carbon Management
- Breakout #4: Energy Storage
- Breakout #5: Energy Materials

1:00 p.m. **AI for Energy Workshop Report: Writing Session**

- *Breakout Leads / Co-leads*

3:00 p.m. **Workshop Concludes**

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AC. ACRONYMS AND ABBREVIATIONS

ACRONYMS	ABBREVIATIONS
AE	applied energy
AI	artificial intelligence
Argonne	Argonne National Laboratory
CDR	carbon dioxide removal
CH_4	methane
CO_2	carbon dioxide
DAC	direct air capture
DFT	density functional theory
DoD	U.S. Department of Defense
DOE	U.S. Department of Energy
DT	digital twin
ECP	Exascale Computing Project
EERE	Energy Efficiency and Renewable Energy (DOE)
EV	electric vehicle
FASST	Frontiers in Artificial Intelligence for Science, Security, and Technology
FECM	Fossil Energy and Carbon Management (DOE)
GHG	greenhouse gas
GIS	geographic information systems
GPU	graphical processing unit
$GtCO_2$	gigatons of CO_2
HFM	high-fidelity modeling
HPC	high-performance computing
INL	Idaho National Laboratory
IRI	Integrated Research Infrastructure
IT	information technology
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LLCF	life-cycle carbon fuel
LLM	large language model
LLNL	Lawrence Livermore National Laboratory
MGI	Materials Genome Initiative
ML	machine learning
NASA	National Aeronautics and Space Administration
NE	nuclear energy
NETL	National Energy Technology Laboratory
NH_3	ammonia
NIST	National Institute of Standards and Technology
NNSA	National Nuclear Security Administration
NRC	U.S. Nuclear Regulatory Commission
NREL	National Renewable National Laboratory
ORNL	Oak Ridge National Laboratory
PMU	phasor measurement unit
PNNL	Pacific Northwest National Laboratory
PSC	point source capture
R&D	research and development

ACRONYMS	ABBREVIATIONS
ROVI	Rapid Operational Validation Initiative
Sandia	Sandia National Laboratories
SME	subject matter expert
V&V	verification and validation

AD. REFERENCES BY CHAPTER

01. Nuclear Energy

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