



U.S. DEPARTMENT OF ENERGY

Genesis Mission

National Science and

Technology Challenges



U.S. DEPARTMENT *of* ENERGY

Contents

Reenvisioning Advanced Manufacturing and Industrial Productivity.....	1
Reimagining Construction and Operation of Buildings	2
Scaling the Biotechnology Revolution.....	3
Securing America's Critical Minerals Supply.....	4
Delivering Nuclear Energy that is Faster, Safer, Cheaper.....	5
Accelerating Delivery of Fusion Energy	6
Transforming Nuclear Cleanup and Restoration.....	7
Discovering Quantum Algorithms with AI.....	8
Realizing Quantum Systems for Discovery	9
Recentering Microelectronics in America.....	10
Securing U.S. Leadership in Data Centers	11
Accelerating Materials Discovery, Production, and Qualification for Strategic Deterrence	12
Achieving AI-Driven Autonomous Laboratories	13
Designing Materials with Predictable Functionality.....	14
Enhancing Particle Accelerators for Discovery	15
Unifying Physics from Quarks to the Cosmos.....	16
Predicting U.S. Water for Energy	17
Scaling the Grid to Power the American Economy.....	18
Unleashing Subsurface Strategic Energy Assets.....	19
Accelerating Nuclear Threat Assessment, Preparedness, and Response.....	20
Harnessing America's Historic Nuclear Data and Research	21
Increasing Experimental Capacity at Nuclear Research Facilities	22
Integrating Design and Production Operations for Nuclear Deterrence	23
Safeguarding Nuclear Materials from Proliferation Threats	24
Streamlining Production, Removing Red Tape, and Ensuring Safety in the Nuclear Enterprise	25
Strengthening Deterrence Through Attribution of Nuclear and Radiological Signatures.....	26

Reenvisioning Advanced Manufacturing and Industrial Productivity

Challenge: Bridging the gap between scientific discovery and commercially viable products and processes, known as the “valley of death”, remains the biggest challenge in industrial manufacturing. The scaling, modification, or deployment of innovative materials and processes depends on a vast and complex parameter space, requiring the uncovering and integration of underlying physical and chemical principles that hold the key to the next United States (U.S.) manufacturing revolution.

AI Solution: Recent advancements in agentic and generative artificial intelligence (AI) present opportunities to accelerate discovery and translational science. These new tools could navigate multi-scale and high-dimensional dynamic systems to find hidden relationships and uncover new manufacturing routes and products. AI can also enable end-to-end digital transformation of industrial manufacturing through integration of real-time data from machines, products, processes, and supply chains into digital twins for continuous human-in-the-loop automated decision support and deployment of emerging advanced manufacturing technologies.

Justification: The U.S. Department of Energy (DOE) National Laboratories co-locate world-leading expertise in the discovery, optimization, and scale-up of novel chemistry and materials for energy applications and in smart manufacturing, as well as operate cutting edge synthesis and characterization facilities and high-performance computing (HPC) resources. At the same time, DOE has a long history of partnering with industry, which has helped cultivate data from industrial facilities. This creates an ideal environment to advance AI-driven manufacturing for U.S. industries today and in the future.

National Impact: Delivering innovations through an efficient, distributed, and adaptive platform capable of real-time decision making and end-to-end intelligence will profoundly transform how we create chemicals and materials foundational to industrial products and advanced energy technologies while strengthening supply chain resilience and competitiveness of American industry to create jobs and economic growth.

Reimagining Construction and Operation of Buildings

Challenge: Building construction faces high costs and long timelines due to fragmented permitting and poor data interoperability. Then, when buildings are operational, sometimes faulty building controls can cause increased energy bills.

AI Solution: AI can transform the entire building lifecycle from design through operation by enabling breakthroughs in automated design, physics-based modeling, rapid permitting, and optimized maintenance. DOE will partner with machine learning and agentic platform developers, and collaborate with building owners, laboratories, construction companies, and others with data that can help validate and accelerate learning.

Justification: DOE's buildings expertise and national laboratory building science capabilities, along with its integrated building research infrastructure and public-private partnerships, make it uniquely suited to tackle this challenge.

National Impact: This effort will reduce construction timelines and costs, increasing housing availability and affordability while making homes and commercial buildings less costly to operate.

Scaling the Biotechnology Revolution

Challenge: Designing biology on demand to innovate in biotechnology and re-establish U.S. leadership will require accurately defining the essential governing principles—from atoms to molecules to organisms to ecosystems and back. However, the nonlinear complexity of biological systems and long, costly development cycles hinder biotechnological innovations, impeding the delivery of crucial biofuels, biochemicals, and bioproducts vital for American economic prosperity and energy independence.

AI Solution: AI will integrate and interpret genomics, multi-omics, imaging, dynamics, and phenomics data into embedded models to establish genotype–phenotype relationships, identify causal control points, and guide autonomous experimentation. This will advance AI's ability to reason about long causal chains under uncertainty, integrate across multiple scales, and learn from sparse, noisy data. Tools like digital twins could be used to derisk process development, optimization, integration, and scale-up, thereby speeding up industrial production of biofuels, biochemicals, and bioproducts by orders of magnitude.

Justification: DOE is uniquely positioned to leverage its world-class molecular and genomic capabilities of the Lawrence Berkeley National Laboratory's (LBNL) Joint Genome Institute, the Pacific Northwest National Laboratory's Environmental Molecular Sciences Laboratory, the specialized feedstock and conversion capabilities of the Idaho National Laboratory's (INL) Biomass Feedstock National User Facility, the National Laboratory of the Rockies' (NLR) Integrated Biochemical Refinement Facility & Process Development Unit, and the LBNL Advanced Biofuels/Bioproducts Process Development Unit facilities and HPC. These DOE assets, combined with AI tools and digital twins, will enable predictive design of biological processes, products, and systems and rapid scale-up of biomanufacturing.

National Impact: Accelerating AI-driven biotechnology will position the U.S. to establish leadership in the biotechnology revolution by rapidly advancing the continuum from discovery to biomanufacturing scale-up, in areas spanning energy, bio-based domestic sources of critical minerals and materials (CMM), health, agriculture, and biosecurity, and will drive economic growth and job creation across the nation.

Securing America's Critical Minerals Supply

Challenge: America's dependence on foreign supply chains for CMM threatens national security, economic competitiveness, and the deployment of technologies essential for energy independence. Domestic critical mineral production is expensive, complex, and time-consuming, in part because of the many steps to identify, extract, refine, and concentrate from complex, heterogeneous sources across critical mineral supply chains.

AI Solution: AI will revolutionize the entire critical minerals supply chain and development of alternative materials by integrating geophysical data, other fundamental science data, process optimization, cost estimation, and economic modeling into one connected system. Solving this challenge demands an AI that can reason scientifically, can understand complex structure-property relationships, and can design alternatives with different compositions. Physics-based AI offers advanced predictive capabilities to identify alternatives and understand processes underlying critical mineral availability, recovery, refinement, and replacement.

Justification: DOE's existing minerals characterization datasets (e.g., METALLIC, Critical Materials Innovation Hub), combined with DOE national laboratory expertise and DOE-supported efforts in materials science, chemistry, geosciences, biology, process engineering, and economic modeling, could enable acceleration from the years-long mineral development timelines to rapid resource assessment and production optimization. Further, use of AI could reveal new strategies to replace and/or eliminate the need for CMMs in some materials and chemical processes.

National Impact: This effort will reduce reliance on adversarial nations, expand America's mineral resource base, maximize production profitability, and strengthen supply chain resilience for technologies essential to national security and economic prosperity.

Delivering Nuclear Energy That is Faster, Safer, Cheaper

Challenge: Nuclear power plants have historically been challenged by long development timelines and burgeoning costs, limiting America's ability to deliver affordable, resilient, and reliable energy as demand continues to grow—particularly from AI data centers.

AI Solution: This initiative will accelerate nuclear energy deployment by using AI to design, license, manufacture, construct, and operate reactors with human-in-the-loop workflows, enabling at least 2x schedule acceleration and greater than 50% operational cost reductions. To meet these goals, we are using a suite of explainable AI solutions including surrogate models, agentic workflows, autonomous labs, and digital twins. For example, for reactor operations, we will use digital twin systems with AI components that will interpret complex operational data in real time.

Justification: DOE's combination of national laboratory nuclear expertise, test facilities (e.g., INL's Advanced Test Reactor, Transient Reactor Test Facility, Fuel Conditioning Facility, Hot Fuel Examination Facility, and Collaborative Computing Center; Oak Ridge National Laboratory's High Flux Isotope Reactor; Argonne National Laboratory's Mechanisms Engineering Test Loop Facility), decades of operational data, regulatory partnerships, industry partners, and extensive computational ecosystem uniquely position it to accelerate reactor deployment.

National Impact: This challenge will provide Americans more affordable energy while reducing human error, strengthening national security, and directly supporting U.S. energy dominance with multi-billion-dollar cost savings per gigawatt of generating capacity.

Accelerating Delivery of Fusion Energy

Challenge: Realizing fusion energy on the grid requires coordinated progress across six tightly coupled challenge areas defined in the Fusion Science and Technology Roadmap.¹ Isolated, device-specific trial-and-error approaches cannot manage these interdependencies at the scale, complexity, or pace required to meet national energy objectives.

AI Solution: AI enables physics-constrained digital twins that integrate plasma, nuclear, materials, and system behavior within a unified predictive framework, allowing performance and engineering trade-offs, failure modes, and design margins to be evaluated consistently in simulation and experiment. An AI-Fusion Digital Convergence Platform (DCP) will integrate novel algorithms in HPC codes, foundation models for plasma and materials science, physics- and chemistry-informed neural networks, surrogate models, and digital twins for whole-facility modeling and real-time control across the six Roadmap challenge areas. The DCP will accelerate infrastructure development, shorten innovation cycles, and support a competitive U.S. fusion ecosystem.

Justification: DOE uniquely brings together fusion facilities, national laboratories, leadership-class computing, data stewardship, and public-private partnerships to build and operate a trusted, national-scale AI platform that integrates data, models, and experiments across the fusion ecosystem. That platform will leverage large-scale domestic and international fusion facilities and fusion materials and technology infrastructure including high-heat-flux testbeds, tritium and blanket test stands and loops, irradiation facilities, and in situ and in operando materials characterization capabilities across both public and private sectors to meet fusion roadmap milestones.

National Impact: The DCP would accelerate delivery of fusion energy as a source of firm, scalable baseload power, strengthening U.S. energy security and competitiveness.

¹ The Fusion Science and Technology Roadmap is available at energy.gov/fusion-energy.

Transforming Nuclear Cleanup and Restoration

Challenge: DOE's environmental cleanup mission faces an estimated \$540 billion liability over eight decades with ~90 million gallons of highly radioactive tank waste requiring treatment that impedes site remediation and restoration crucial for American energy, security, and innovation.

AI Solution: A multimodal AI foundation model will be trained on DOE Office of Energy Management's (EM) unparalleled 30+ years of operational data from unique nuclear processing facilities to predict scale-dependent behavior across lab, pilot, and full-scale systems. National laboratory experts will leverage Equinox supercomputing capabilities for accelerated simulation architecture in development of the AI models. The goal is to use AI to enable mission acceleration to meet EM's 2040 vision with significant liability reduction.

Justification: DOE EM's unique data assets from designing and operating large-scale facilities at complex sites (e.g., the Defense Waste Processing Facility and the Salt Waste Processing Facility at the Savannah River Site (SRS)), combined with the capabilities provided by the industry partners, will enable development of scale-bridging AI models that safely and efficiently address deployment challenges (e.g., the Waste Treatment and Immobilization Plant at the Hanford Site) no other institutions can leverage.

National Impact: This transformation will compress deployment timelines and accelerate nuclear remediation, thereby enabling renewed use of nuclear materials (for energy and medical applications) and infrastructure for American energy dominance.

Discovering Quantum Algorithms with AI

Challenge: Discovering new quantum algorithms is an exceptionally difficult challenge due to the number of potential quantum operations and is highly counter-intuitive for human researchers to navigate. U.S. leadership in the emerging quantum computing revolution will require accelerating the design and development of quantum algorithms (including those that capitalize on the convergence of classical HPC, AI, and quantum computers) that demonstrate scientific utility and a provable quantum advantage.

AI Solution: Novel AI could discover new quantum algorithms by automating and optimizing their design and translating them into applications without requiring prior domain knowledge. Furthermore, AI-powered platforms can translate high-level problem descriptions in natural language into executable quantum circuits, making algorithm design more accessible to researchers from various fields. AI could help establish scientific workflows that leverage the interplay of classical and quantum resources, managing data flow and executing complex computations across platforms.

Justification: There is strong evidence that quantum computers and algorithms will offer solutions to computational problems with high impact to the scientific community, beyond the limits of classical HPC and AI. DOE hosts the most complete suite of scientific computing capabilities and these advances in quantum capability will enable computations that are classically intractable.

National Impact: The discovery of new quantum algorithms will have broad applications to science domains, such as fusion sciences, high energy physics, nuclear physics, materials science, and chemistry, with proposed commercial applications for the acceleration of drug, material, and chemical discovery. This technological leap would not only bolster the nation's economy and security but also provide tools to address some of the most challenging scientific and societal problems.

Realizing Quantum Systems for Discovery

Challenge: Quantum systems for quantum computing, quantum sensing, and quantum communication are poised to revolutionize discovery science by enabling unprecedented capabilities in modeling, simulation, and measurement. The use of current quantum systems is severely limited by their fragility, scalability, and integration into existing infrastructure. The inherent challenge is the lack of understanding and control of the complex cause-and-effect relationships within a quantum system.

AI Solution: AI has shown its ability to process vast amounts of multimodal data, to recognize complex patterns and relationships, and to learn adaptively how to handle dynamic and unpredictable environments. This ability makes AI uniquely suited to help understand and control the delicate nature of complex quantum systems. In quantum computing, AI will assist in real-time noise mitigation, adaptive error detection and correction, and system optimization and design. In quantum sensing, AI will optimize quantum entanglement, increase sensitivity, and control multi-sensor quantum networks. In quantum communication, AI will dynamically optimize multi-node quantum network design and control. New AI approaches are needed for making real-time decisions under quantum uncertainty, learning control policies when observation is costly and destructive, predicting behavior from incomplete information, and adapting to drift in real-time.

Justification: DOE is home to five National Quantum Information Research Centers in the U.S. working on overcoming limitations in quantum computing, quantum sensing, and quantum communication. The existing ecosystem is ideally suited to develop AI solutions to enable full quantum control.

National Impact: The AI enabled understanding and control of complex quantum systems will accelerate the deployment of quantum technologies and accelerate their utilization for currently intractable challenges in scientific discovery and technology development.

Recentering Microelectronics in America

Challenge: Microelectronics powers all aspects of our lives, including AI, but America faces intense global competition in critical microelectronics applications, including ultra-efficient semiconductors for AI computing, power electronics, and communication networks. Microelectronics faces a tremendous scientific and technological challenge: designing and engineering the next generation of microelectronic devices and platforms that push the boundaries of miniaturization, processing speed, power consumption, thermal management, and operations environment.

AI Solution: An AI-driven full-stack co-design ecosystem will enable faster innovation cycles, de-risk new ultra-efficient manufacturing processes and component designs, and accelerate materials and manufacturing research and development (R&D), thereby leapfrogging foreign semiconductor technology. Frontier AI coupled with heterogenous and multiscale data that is accessible via federated learning techniques will accelerate microelectronics research by revealing the critical relationships and tradeoffs between materials, devices, and workflows.

Justification: For decades, DOE has been at the leading edge of microelectronics research, both as a consumer and as an engine of scientific innovation with expertise in advanced materials, nanofabrication, and quantum-related technologies such as cryogenics, enabling many of the technological breakthroughs adopted by industry.

National Impact: Microelectronics continues to be at the heart of technological innovation, and every American will benefit from recentering leadership of the industry in the U.S. This effort will ensure sustained U.S. leadership in the global semiconductor landscape, enabling the rapid growth of domestic data centers, advancing beyond Moore's law for AI computing and national security applications, and securing other technological advantages—such as global leadership in 6G communication networks essential for economic prosperity and national security.

Securing U.S. Leadership in Data Centers

Challenge: Winning the AI race will require accelerating the process of developing and deploying new data center technologies and energy management strategies to provide the extreme compute power for AI advancements, while ensuring secure, reliable, and affordable energy for consumers.

AI Solution: By leveraging AI/machine learning (ML), digital twins, and cyber-physical testbeds, we can rapidly de-risk advanced data center technologies and their grid integration, accelerating the time to deployment and supporting stakeholder needs including data center operators, equipment providers, communities, and utilities. AI/ML can accelerate physics-based models to enable real-time digital twins, explore millions of deployment scenarios, and optimize under a unique constraint surface.

Justification: This project leverages DOE's capacity to convene data center and utility stakeholders, the national laboratories' research expertise in both load flexibility and computing, and their unique cyber-physical testbed facilities. Specifically, the DOE already supports the Center of Expertise for Data Center Energy at LBNL, which can provide resources, including a variety of data sets on data center energy use, to aid this effort.

National Impact: By ensuring a robust capacity to develop cutting edge data center technologies and load management strategies, we will solidify U.S. intellectual and economic leadership in AI, driving prosperity and security while maintaining secure, reliable, and affordable energy for consumers.

Accelerating Materials Discovery, Production, and Qualification for Strategic Deterrence

Challenge: The nuclear security enterprise faces significant hurdles in discovering, manufacturing, and qualifying mission-critical nuclear and non-nuclear materials. This challenge will develop a digital, AI-accelerated workflow that connects the entire lifecycle of critical materials, from initial formulation to final production. This approach will incorporate real-time anomaly detection and in-process corrections to significantly reduce the need for extensive qualification testing and improve the safety and reliability of these critical materials. It will also expedite new materials development, enabling opportunities to meet evolving military requirements.

AI Solution: Develop an AI-driven workflow that links material design, automated testing, and qualification into a single, data-driven process by using physics-based simulations on high-performance computers to screen and optimize material candidates, directing robotic labs and in-line sensors to run experiments, feed results back, and refine virtual performance models, and automatically assembling risk-based qualification packages that can be shared across sites for fast, coordinated approvals. This workflow also includes automated AI agents that invent and test new plutonium purification methods and deliver only the best options to scientists for review, compressing a months-long development process into just days.

Justification: The National Nuclear Security Administration (NNSA) uniquely combines supercomputing power, specialized test facilities, and decades of mission data. By uniting these assets in an AI-managed pipeline, we can shrink discovery-to-qualification times, improve manufacturing reliability, and build a stronger domestic supply of critical materials—without sacrificing safety or oversight.

National Impact: Accelerating material development and certification will ensure the timely delivery of strategic components for deterrence, reduce reliance on fragile supply chains while lowering overall program costs, and provide a scalable model for safer, more efficient manufacturing in civilian sectors such as energy, chemicals, and aerospace.

Achieving AI-Driven Autonomous Laboratories

Challenge: The pace of scientific discovery is influenced by the traditional, human-driven experimental process and the availability of non-deterministic AI-driven control tools to implement complex experimental designs in combinatorially large design parameter spaces. These bottlenecks slow the cycle of hypothesis, experimentation, and discovery, leading to inefficient use of critical national assets and delaying scientific breakthroughs. Automating at least some parts of the scientific experimental scheme will both increase the volume of data produced for improved AI models and improve the repeatability of experiments.

AI Solution: Artificial intelligence will be integrated directly into the experimental workflow and data analysis, combining robotics, edge AI, real-time analysis and intelligent feedback, hypothesis generation, and data curation/sharing.

Justification: These AI-driven laboratories will allow scientists to explore complex phenomena at an unprecedented rate and scale and are critical to achieving the Genesis Mission goals. DOE's user facilities and long-standing national laboratories have the infrastructure, capabilities, and expertise to serve as the nucleus for innovation with this type of high throughput discovery.

National Impact: Accelerating discovery through AI-driven laboratories will directly advance U.S. scientific leadership and economic competitiveness. This capability will speed up the development of novel materials and molecules for energy, next-generation computing, national security, and biotechnology. Like other challenges, it will also solidify the nation's position at the forefront of AI and scientific innovation, create a new paradigm for 21st-century research, and train a future workforce fluent in the integration of AI, data science, and experimentation.

Designing Materials with Predictable Functionality

Challenge: Accelerating materials innovation will enable rapid deployment of advanced energy and industrial technologies that are essential for American competitiveness, from structural materials to materials for energy storage to other functional materials for advanced technologies. The identification and commercialization of new materials with transformative properties that dramatically improve performance, energy efficiency, reliability, and resilience, however, is a time- and resource-intensive process due to the inherent complexity of materials science and the practical limitations of traditional simulations, synthesis, and characterization techniques that still require significant trial and error.

AI Solution: The convergence of current and emerging AI technology with the growing availability of large, curated datasets may be a tipping point for materials discovery, design, and qualification. The development of physics-aware AI frameworks that exploit the complementary strengths of foundation models, deep learning, computer vision, generative AI, and agentic AI will enable entirely new capabilities for materials design that iteratively couple prediction, synthesis, characterization, and analysis to yield closed-loop learning systems that are interpretable, trustworthy, and capable of bridging large scales in space and time. The ultimate goal of inverse design (designing materials for given property specifications) requires advanced experimental and simulation capabilities as well as AI reasoning and explainability.

Justification: DOE's suite of world leading and unique experimental and computational capabilities for materials research, including X-ray light sources, neutron scattering facilities (and their associated characterization equipment), nanoscale science research centers, materials databases, and exascale computers, is collectively the most comprehensive and performant in the world. These capabilities, along with the availability of very large materials data sets coupled with sustained investments in the development of AI-enabled physics-informed models, has positioned DOE to take a leadership role in implementing the materials by design vision.

National Impact: Tight integration of AI into the materials discovery-to-product workflow could significantly reduce time to market in manufacturing—from many years to decades down to months to a few years. This acceleration will dramatically reduce development timelines for critical technologies including batteries, energy systems, structural and functional materials, strengthening American technological leadership and enabling faster deployment of innovations that create jobs and strengthen economic and national security.

Enhancing Particle Accelerators for Discovery

Challenge: Modern particle accelerators are complex, requiring extensive human intervention that leads to high operating costs, operational variability, suboptimal experiment optimization, and inadequate data integration. Further, the physical limitations of existing accelerator technologies slow progress in pushing the limits of resolution in space, time, and energy. Transforming accelerator-based facilities into highly efficient, autonomous, and more productive capabilities requires a tight integration of AI with design and operation.

AI Solution: Predicting chaotic beam dynamics, in which small perturbations cascade into major problems, could push AI to develop new capabilities in multi-scale temporal reasoning, physics-constrained learning, and robust uncertainty quantification. AI-driven digital twins that simulate complete beam dynamics in real time could dramatically reduce tuning time. Collectively, facility-based AI will become adaptive and self-updating, significantly boosting performance, efficiency, and scientific output.

Justification: DOE stewards one of the largest suites of accelerator-based experimental facilities in the world, with extensive operational data and a large, highly skilled workforce. The optimization of the nation's large-scale scientific infrastructure through AI-enabled design and the elimination of operational bottlenecks and cost inefficiencies will maximize the nation's return on current and future infrastructure investments, revealing entirely new paradigms for scientific research through human-AI teaming and accelerating discovery.

National Impact: Accelerator-based facilities have been central to many of the most important discoveries of the 20th and 21st centuries. Integrating AI into accelerator design and optimization will increase the pace of future breakthroughs, enabling a deeper understanding of the universe, the development of new energy and computing technologies, and the creation of new techniques for the diagnosis and treatment of disease.

Unifying Physics from Quarks to the Cosmos

Challenge: The universe obeys only one set of rules, and scientists have hundreds of experiments targeting parts of that one set. Experiments range over distance scale (31 orders of magnitude), cost (\$100k to \$B), duration (fractions of a second to decades), and human investment (few to thousands). We need a way to integrate the disparate experimental results with theoretical knowledge to accelerate discovery.

AI Solution: High-energy physics and nuclear physics form a unique foundation to build AI reasoning models at unprecedented scale. Developing AI that simultaneously learns from particle collisions, nuclear decays, and cosmological surveys will require breakthroughs in multi-modal learning and the ability to derive insights rather than merely recognize patterns. An AI that internalizes the Standard Model could accelerate analysis by orders of magnitude, identify anomalies pointing to new physics, and propose theoretical extensions consistent with all data—a leap from pattern matching to physics reasoning.

Justification: DOE uniquely possesses the confluence of world-class scientific talent, stewardship of cutting-edge facilities, unparalleled access to experimental data, and a critical national mission to effectively address this challenge. These facilities, alongside a broad portfolio of programs that explore the fundamental constituents and forces of the universe and delve into the nature of atomic nuclei, underscore DOE's singular ability to conduct large-scale, long-term, and high-impact scientific research.

National Impact: The acceleration of discovery, particularly in areas involving vast datasets from cutting-edge experiments, means we could reach breakthroughs much faster than previously possible, impacting our technological capabilities and quality of life in unforeseen ways. Questions such as why is there more matter than antimatter, what is the nature of dark matter, and how do protons generate mass and spin address the nature of reality, and answering questions through advanced AI could have profound shifts in our philosophical and scientific understanding of the cosmos and our place within it.

Predicting U.S. Water for Energy

Challenge: Water availability is essential for expanding production and utilization of energy, as well as the nation's health and security. However, there are fundamental scientific gaps in our understanding of terrestrial and atmospheric systems that limit our ability to predict water resources, especially on the time scale of weeks to years.

AI Solution: AI capable of multi-scale temporal reasoning could tackle three inter-related grand challenges: cloud physics, surface and subsurface water flows, and the broader hydrologic cycle. AI could improve, accelerate, and couple exascale-class modeling systems through advances in model initialization, and develop surrogates trained on DOE's atmospheric and terrestrial observations and laboratory data, at a fraction of the computational cost of existing models. AI-based model diagnostics for enhanced analysis could refine a model-observational system aligned with decision-making needs.

Justification: DOE is the only agency with AI expertise, advanced computing, and integrated modeling capabilities (e.g., the DOE Energy Exascale Earth System Model, or E3SM), and infrastructure for field research necessary to meet the challenge of providing accurate information on surface and ground-water availability on the time scales of weeks to years.

National Impact: Solutions to these longstanding science challenges will radically improve America's ability to anticipate water supply in the context of changing water availability, demands, energy technologies, and ambitions for energy expansion.

Scaling the Grid to Power the American Economy

Challenge: The electric grid faces reliability challenges and infrastructure limitations to accommodate dramatic increases in electricity demand from data centers, manufacturing, and electrification while maintaining affordable power for Americans.

AI Solution: AI, using deep and reinforcement learning techniques on newly integrated big data sources, will reduce uncertainty, improve insights, and speed processes in grid planning, interconnection, operations, and security. This effort aims to enable 20-100x faster decision-making and at least 10% improvement in electricity cost and reliability.

Justification: The utility sector has critical grid data but a low risk tolerance, limited ability to develop new technology, and regional focus. DOE can bring integrated energy system expertise, computational facilities, and testbed infrastructure like the Critical Infrastructure Test Range Complex (CITRC) at INL and the Advanced Research on Integrated Energy Systems (ARIES) platform at NLR. The Department's strong partnerships with grid operators can bring utility data together with these DOE capabilities to develop validated, deployable AI solutions.

National Impact: This modernization will deliver lower-cost, more reliable power to American homes and businesses while strengthening energy security through faster deployment of grid capabilities and improved resilience against threats.

Unleashing Subsurface Strategic Energy Assets

Challenge: Delivering cost-effective energy from the Earth's subsurface entails the use of heterogeneous reservoirs, dominated by fractures. Tools capable of predicting reservoir behavior and the interactions of complex biogeochemical, mechanical, and hydrologic processes are critical to the development of innovative, cost-effective extraction of subsurface energy sources, including unconventional oil and gas, geothermal, and coal bed methane.

AI Solution: Developing AI capable of reasoning under extreme uncertainty, integrating heterogeneous data types (i.e., seismic, geochemical, biological, hydrologic), and building predictive models of systems that cannot be directly observed has broad applicability to any domain requiring inference from indirect evidence. For subsurface science, AI that connects molecular-scale mechanisms to field-scale resource availability will transform the field from descriptive to predictive. DOE's vast biological, geochemical, geomechanical, and hydrologic data sets can be combined with high performance modeling capabilities, laboratory analytics, and a suite of AI technologies, including surrogate models, physics-informed machine learning, and digital twins to enhance engineering evaluation and control of the subsurface during characterization, drilling, stimulation, and production.

Justification: DOE's laboratory complex includes a vast array of data, modeling, and analytical capabilities (e.g., Science-informed Machine Learning for Accelerating Real-Time Decisions in Subsurface Applications (SMART) Initiative suite of tools and machine learning-based surrogate models; National Energy Technology Laboratory's Energy Data eXchange (EDX) Discover; LBNL's Transport Of Unsaturated Groundwater and Heat (TOUGH) simulation suite; Los Alamos National Laboratory's (LLNL) GeoDTi design tool; LLNL's GEOS software; and PFLOTRAN and ATS models), that supports extensive research and operational activities in subsurface environments, and are uniquely positioned to apply AI to accelerate development of models that emulate microbial, mineral, and fluid interactions across molecular to field scales. Efforts will assemble, train, and analyze information from vast data libraries, experiments, and operational sensors, to produce subsurface transport models and digital twins to enhance reservoir characterization, enable real-time reservoir simulation, and address uncertainty to increase hydrocarbon resource recovery and unlock geothermal resources.

National Impact: Understanding subsurface complexities and stored energy sources is key to securing the nation's energy future and will reduce the costs of recovery for oil, gas, and heat, reduce costs of power to U.S. consumers, re-shore manufacturing, and enhance U.S. competitiveness.

Accelerating Nuclear Threat Assessment, Preparedness, and Response

Challenge: Rapid and effective response to nuclear and radiological events demands detailed analysis of vast and varied data, from radiation detectors and environmental sensors to intelligence reports and simulation outputs. Today, our Nuclear Emergency Support Teams (NEST) rely on manual review and static AI models that cannot sufficiently adapt as new data streams in, creating delays in detection, assessment, and response. This leaves decision-makers without real-time situational awareness or clear risk metrics when addressing threat assessments and event response.

AI Solution: Deploy a continuously learning, multimodal AI fusion system that integrates radiation/environmental sensors, simulations, and intelligence reporting to deliver real-time decision support with scenario modeling and uncertainty-aware risk metrics on crisis timelines.

To accelerate progress, we must develop cross-classification data governance and trusted deployment patterns (edge-capable compute, rigorous red-teaming, and auditable human-approval workflows) so the system can be used operationally without sacrificing reliability.

Justification: NNSA uniquely combines nuclear science expertise, secure facilities, and HPC resources. This effort will embed physics-informed models for transparent, auditable AI in mission-critical environments, replace brittle, hand-tuned workflows with a single scalable solution cutting development time and cost, and leverage existing archives and platforms for rapid deployment and scaling.

National Impact: This system will shrink detection-to-response times from days to hours, enhancing public safety and national security. It will improve decision confidence and reduce false alarms through clear, quantified risk assessments, strengthen deterrence by embedding AI into critical decision loops and supporting interagency coordination, and deliver cost-efficient capabilities that can be adapted by civilian emergency responders and international partners.

Harnessing America's Historic Nuclear Data and Research

Challenge: The United States possesses a vast and unparalleled archive of classified scientific experiments and nuclear weapon tests, as well as unclassified historical work in nuclear science that spans more than eight decades. However, much of this vital information exists only in written notes, printed materials, or photographs, and has yet to be digitized and adequately labeled, hindering its accessibility and usability for continued research, design, and production. This challenge is significant because it addresses the urgent need to modernize historical information and convert it into usable data for enhanced security and research by AI tools. The challenge also addresses the call expressed in the President's Executive Order to make federally owned data sets a key component of the Genesis Mission.

AI Solution: Build an AI digitization-and-reconstruction pipeline (optical character recognition + vision + information extraction + 3D/geometry inference) that converts analog reports, imagery, and drawings into searchable, simulation-ready datasets, including automated meshing and cross-referencing to historic test outcomes. To accelerate progress, we must establish a secure centralized archive with durable metadata/ontology standards, triage workflows that prioritize the highest-value records, and end-to-end access controls and quality assurance processes that function across classification levels.

Justification: The project is critical for preserving valuable historical records and enhancing data management capabilities. It will preserve eight decades of at-risk physical records before degradation or loss, leverage NNSA's secure computing, classification expertise, and specialized archives, and cut manual cataloging effort by an order of magnitude and ensures consistent data quality. Finally, it establishes a compliant, scalable system for ongoing data ingestion and governance.

National Impact: The outcomes of this initiative will significantly enhance research capabilities and support informed decision-making in nuclear stewardship. This initiative will accelerate research and decision-making by unlocking historical test insights, safeguard institutional memory and informs future policy, safety, and treaty verification, and enhance transparency and accountability in nuclear stewardship. This project lays groundwork for broader scientific and security applications of legacy data.

Increasing Experimental Capacity at Nuclear Research Facilities

Challenge: The NNSA is confronted with increasing demand for optimized experiments, conducted at limited-capacity facilities. Current processes to design, document, and analyze experiments are often slow and inefficient, leading to backlogs in experimental campaigns and reduced facility capacity.

AI Solution: Deliver an AI “facility operating system” that uses agentic workflows to plan/schedule experiments, steer execution in real time, and fuse live diagnostics with multi-fidelity simulation so each shot/test yields maximum information with minimal turnaround.

To accelerate progress, we must build interoperable facility digital twins and streaming data/provenance standards, plus transparent approval gates, audit logs, and uncertainty-aware analytics that operators can trust in high-consequence environments.

Justification: NNSA’s integration of advanced technologies and resources uniquely positions it to address important challenges in nuclear security. NNSA combines limited-capacity, high-consequence experimental facilities and test sites with supercomputing, advanced simulation, and automated labs under a secure framework, enabling real-time inference by uniting diverse physics models, uncertainty quantification, and robotic execution. This produces a scalable, reusable architecture (facility models, data standards, and assurance methods) that meets strict safety, security, and quality controls.

National Impact: The outcomes of this initiative extend beyond NNSA, providing broader benefits to nation by increasing experimental throughput and cutting the number of costly physical tests required, speeding time-sensitive stockpile stewardship and deterrence decisions with higher-confidence results, and creating a transferable model for AI-driven R&D and automated operations across aerospace, energy, microelectronics, pharmaceuticals, and other strategic industries.

Integrating Design and Production Operations for Nuclear Deterrence

Challenge: Deterring America's adversaries from using strategic weapons has never been more urgent or more complex. Answering that threat requires greater flexibility and innovation in our nuclear weapons production capabilities. The current handoff of weapons systems between Design Agencies (DAs) and Production Agencies (PAs) is slow and inefficient, hindering our deterrence mission. This initiative will develop an AI-accelerated, model-based systems engineering platform that spans and integrates design and production processes. By leveraging multiscale physics, digital twins, and AI capabilities, NNSA will enhance decision-making, reduce rework, and improve production efficiency to provide new weapons systems to warfighters in a fraction of the traditional time and cost.

AI Solution: Deliver an AI-powered "nuclear security enterprise twin" that couples physics-constrained surrogates, production digital twins, and agentic workflows to co-optimize designs and manufacturing in a closed loop—dramatically shrinking DA/PA iteration time while preserving traceability and decision quality.

To accelerate progress, we must build secure cross-site data interoperability (schemas, provenance, and governance), validated and uncertainty-aware models, and human-in-the-loop orchestration with auditable controls that work across required classification environments.

Justification: This initiative is particularly suited to the NNSA because it leverages secure access to extensive historical design and production data, HPC capabilities for developing and validating advanced models, and reliable AI systems that can function across various network classifications.

The result will be nothing short of a revolution in weapons design and production. By creating an AI-integrated Certification Environment, NNSA can shift from traditional document-based processes to agile, model-driven decision-making. This transformation will streamline operations, reduce rework, and ensure alignment between design intentions and production realities as requirements evolve.

National Impact: This initiative aims to enhance national security by revolutionizing collaboration between DAs and PAs, ensuring timely and cost-effective modernization programs. It strengthens national security by accelerating modernization programs on time and within budget, with high confidence in outcomes; provides scalable capabilities and technologies that can be applied to large-scale American industries, including automakers, shipbuilders, aerospace, and microelectronics; and minimizes waste of valuable resources, bolsters domestic manufacturing capabilities, and decreases manufacturing ramp times.

Safeguarding Nuclear Materials from Proliferation Threats

Challenge: Preventing nuclear materials and information from falling into the hands of rogue and dangerous actors (non-proliferation) is central to America's national security. Against the backdrop of a global surge in demand for civilian nuclear power, the challenge of monitoring and enforcing non-proliferation commitments is growing rapidly. To effectively investigate and prosecute potential threats, we integrate vast amounts of complex data from diverse sources using AI. This challenge will develop and deploy advanced AI technologies that can analyze these growing data streams in real time, identifying anomalies that indicate potential proliferation activities. This will not only enhance and speed our enforcement against proliferation activities but will further strengthen America's deterrent by discouraging bad actors from even attempting to circumvent and defeat international controls of nuclear materials and information.

AI Solution: Develop multimodal foundation models and analytic agents that fuse satellite imagery, sensing, open-source, and government data to detect subtle proliferation-relevant anomalies in near real time and generate analyst-ready evidence packages with confidence scoring.

To accelerate progress, we must build secure multi-network data-sharing and governance, domain ontologies and knowledge graphs for the fuel cycle, continuous testing and red-teaming, and human-AI teaming interfaces that scale across classified and unclassified environments.

Justification: The project leverages NNSA's unique capabilities to address the challenges of modern data analysis in nonproliferation efforts. NNSA is the only organization with the nuclear fuel cycle domain expertise required to aggregate global nonproliferation-relevant data sources. Manual analysis cannot keep pace with the volume and variety of modern data streams; automated, trustworthy AI shortens detection timelines, increases efficacy of detection activities, and improves use of technical subject matter experts. This effort will leverage existing and planned NNSA platforms and partnerships for rapid deployment.

National Impact: The outcomes of this initiative will significantly enhance U.S. national security and global nonproliferation efforts by accelerating threat detection and decision cycles, strengthening U.S. deterrence posture. It will provide policymakers with timely, credible intelligence to guide diplomatic and enforcement actions, enhance global nonproliferation cooperation by sharing standardized, auditable insights, enhance the perceived and real value of cooperation with America on civilian nuclear activities, and establish a model for AI-driven monitoring in other critical security domains.

Streamlining Production, Removing Red Tape, and Ensuring Safety in the Nuclear Enterprise

Challenge: Not all challenges to our nuclear deterrence are external; some are directly within our own walls. Current regulatory processes in high-hazard facilities are slow and fragmented, leading to inefficiencies that can compromise safety and operational effectiveness. These mostly well-intended policies are no longer compatible with the urgency of NNSA's modernization and production mission. This challenge is significant as it directly impacts the ability to respond to nuclear threats as well as to maintain safety standards efficiently. AI-driven facility and process models can optimize operations with real-time data to streamline schedules, allocate resources, and eliminate bottlenecks.

AI Solution: Deploy auditable, policy-grounded AI (large language models + agents) that can digest safety-basis requirements, automate safety analyses and documentation, and continuously generate risk-aware work plans while autonomously configuring and running large simulation campaigns.

To move faster safely, we must establish a trusted digital regulatory corpus with provenance, develop verification and testing harnesses for AI outputs, and integrate these tools into facility/operations data systems with robust access controls and end-to-end audit logs.

Justification: The project is designed to enhance safety and efficiency by providing transparent, auditable AI solutions that support expert oversight in critical operations. It transforms compliance into a strategic advantage; by digitizing and AI-enabling regulatory documents in situ, we create a verifiable, fully auditable record of every search, analysis, and decision, turning safety basis navigation from a bottleneck into a transparent trust-building capability. The effort ensures data-driven efficiency, unifying engineering, safety, and operational data to cut planning and documentation time by over 50%. Finally, it leverages existing strengths by building on secure data networks and in-house expertise to rapidly deploy and validate advanced AI tools.

National Impact: The outcomes of this initiative will significantly benefit national security and the broader American industry by improving operational efficiency and reducing costs. It will provide faster delivery of manufactured components by accelerating planning and safety reviews while maintaining rigorous safety standards, relevant for NNSA and American industry more broadly. This initiative will also save costs and reduce waste with fewer rework cycles and lower documentation overhead that save taxpayer dollars and conserve critical materials. Finally, it will serve as a scalable model for industry by leveraging transferable methods that boost efficiency and safety in civilian nuclear energy, chemical processing, and aerospace.

Strengthening Deterrence Through Attribution of Nuclear and Radiological Signatures

Challenge: Every nuclear material has a signature. Through a combination of radiological and material characterization analysis, the provenance of loose or employed nuclear materials (like with a weapon of mass destruction or a dirty bomb) can be positively determined. Deterrence is only possible if the very real threat of American retaliation can hold adversaries accountable for their actions. Therefore, the challenge of attributing nuclear materials outside of controlled environments is critical for national security. This effort will dramatically improve the speed and accuracy of nuclear forensics analyses by removing uncertainty or anonymity from the misuse of nuclear materials, thereby enhancing deterrence against potential nuclear threats. This initiative aims to leverage AI to drastically accelerate nuclear forensics in off-normal, uncontrolled, and novel environments.

AI Solution: Field multimodal forensic AI (vision + spectroscopy + morphology + inverse modeling) that can rapidly characterize samples and debris, infer likely process history/origin, and support device/material reconstruction while enabling portable, on-site triage tools.

To accelerate progress, we must build curated and shareable signature libraries with ground-truth links, standardized lab-to-field workflows with calibration and uncertainty quantification, and validated deployment pipelines that preserve chain-of-custody, auditability, and expert oversight.

Justification: The project capitalizes on NNSA's unique resources and expertise to enhance the speed and accuracy of nuclear threat attribution. It builds on NNSA's unique combination of nuclear test archives, specialized labs, and expert staff, eliminates current multi-day bottlenecks in sample processing and reporting, resulting in more efficient use of existing resources, directly supports the deterrence of nuclear threats by enabling fast, credible attribution, and leverages existing infrastructure investment for rapid implementation without compromising quality.

National Impact: The outcomes of this initiative will significantly improve national security and public safety by accelerating threat assessment processes. It will shrink the timeline from material collection to attribution, accelerating policy and response decisions; reinforce deterrence by showing adversaries that misuse of nuclear materials will be traced swiftly leading to decisive American retribution; enhance public safety through faster, more reliable threat assessments and disaster response; and create AI-based forensic methods that can be adapted to other critical security and industrial domains.



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