FUTURE SCIENCE & TECHNOLOGY OPPORTUNITIES

NATIONAL LABORATORY DIRECTORS COUNCIL

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The Department of Energy (DOE) national laboratory system was borne out of the Manhattan Project after World War II to address major challenges facing our nation and the globe. Recognition of the pivotal role that rapid advances in science and technology, aligned to national needs, played in World War II led to a new type of institution, a National Laboratory. The National Laboratories' research and development (R&D) role is never more important than today, given the rapidly evolving global landscape.

Our world and nation face profound challenges in producing clean energy and water, mitigating and adapting to climate change, ensuring security, and enhancing human health. Countries that are successful in meeting these challenges will secure vibrant economies and high standards of living. We must address risks created by natural and man-made threats and rapidly respond to technological surprises. To be prepared, a multi-decade effort is needed for R&D across all scientific and engineering disciplines, deployment of new technologies, and new policy frameworks. We need an enhanced focus on partnerships linking universities, national laboratories, government, and industry. And there is a robust and sustained science and innovation agenda that must be defined to address these global and national challenges.

DOE's National Laboratories together are a national intellectual asset and set of R&D facilities that serve the United States remarkably well and are envied and emulated by other countries. They tackle large-scale, long-term R&D challenges as an interdependent system with distinctive capabilities and world-leading staff and facilities. They have delivered the science and technology (S&T) needed to solve problems of national and global importance, producing a wealth of discoveries and innovations in support of DOE's overarching mission of advancing the national, energy, and economic security of the United States. The laboratories also are relied upon to deliver rapid-response science and technology to help respond to natural and man-made threats and disasters (e.g., Fukushima, Deepwater Horizon, Hurricane Katrina, Superstorm Sandy, Puerto Rico earthquake, Ukrainian grid cyber-attack, and COVID-19).

The National Laboratories occupy a unique niche in our country's R&D ecosystem. They complement the roles and capabilities of academic and industrial research efforts. They independently and collaboratively conduct mission-driven, crosscutting, and often high-risk and hazardous R&D that requires unique instrumentation and facilities that would be ill-suited to an educational institution or beyond the risk tolerance of a corporate research lab. Of course, the laboratories do not operate in isolation. On one hand, they collaborate with universities in fundamental and applied research and support the training of thousands of future scientists and engineers. On the other hand, the laboratories partner with industry and other branches of government in technology development and deployment to ensure the transfer of their R&D to the marketplace. These partnerships result in S&T workforce development and near- and long-term economic impacts through job creation and technology transfer.

Given our important and sustained role as a leader and lynchpin for the nation's S&T ecosystem, the directors of the 17 National Laboratories embarked on an effort to define a small set of multidisciplinary, broad, high-impact, forward-looking (20 to 30-year horizon) S&T opportunities to better address the challenges facing our world and nation. The five opportunities leverage the foundational S&T capabilities maintained by the laboratories. They think beyond current programs and require a whole-of-government approach, which the National Laboratories are uniquely positioned to contribute to. The five opportunities are the future of biotechnology and the future bioeconomy, the future of accelerator science, technology, and engineering, the future of deterrence, the future of computing, and the future of energy systems. These S&T opportunities are critical and urgent, and will be transformational and disruptive, leading to scientific and engineering breakthroughs in many areas of human health, environment, energy, and security.

The five S&T opportunities are described below (not in priority order). Each is outlined in detail along with discussion of why it is important in addressing global and national challenges. The 17 directors look forward to engaging leaders in science and innovation, government, and industry to further develop our ideas and implement a robust R&D agenda over the coming decades focused on significant global and national challenges.

I. The Future of Biotechnology and the Future Bioeconomy: Convergence and the Impact of Rapidly Advancing Technologies

STATEMENT OF THE OPPORTUNITY

Many have deemed the 21st Century as the age of biology, celebrating that it has the potential to contribute practical solutions to many of the major challenges confronting the United States and the world, including the current pandemic. A growing population requires advancements in energy, food, water, and sustainable materials. Rapid progress in the understanding of complex biological systems and in new technologies is transforming and accelerating the practice of biology and its myriad applications. Notably, assessments highlight that these benefits will be derived via closer collaboration with physical, computational, and earth scientists; mathematicians; and engineers.

This convergence science impacts the missions of DOE: New physical science tools enable the key measurements for biology; biological mechanisms are informing physical science problem-solving; and high-performance computing, data science, and artificial intelligence make possible deeper understanding of all complex systems. Energy and environmental restoration are directly aided by the larger, more capable, bio-informed toolsets. And advances in biology have important implications for national security.

DOE should pursue a research initiative focused on the bioeconomy, mission-relevant biotechnology, and agile public-public and public-private collaborative partnerships to accelerate the nation's ability to reap the benefits of the modern biological revolution. The immediate focus should be to apply DOE's technical capabilities and large-team science approach to help limit the deleterious effects of the COVID-19 pandemic. The long-term goal is to make sure the U.S. leads the global bioeconomy, which will help lift the nation out of the economic downturn caused by the pandemic. The DOE's biotechnology effort will continue to be executed in collaboration with other federal departments and agencies as well as universities, private sector partners, and international collaborators.

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Achievement of such an initiative will provide solutions to key societal needs delivered from a robust bioeconomy: sustainable food production, ecosystem restoration and balanced carbon and nutrient cycling, optimized biofuel and bioproduct production, and improved human health. This initiative will ensure availability of the knowledge and tools needed to address future pandemics and other natural and man-made biological threats.

Building on DOE research approaches and outcomes in biology, physics, chemistry, materials science, and precision instrumentation, this effort will aim for multiscale molecule-to-biological system understanding of biological systems within the context of important national objectives. Specifically, the initiative will address the systematic functionalization of biological systems, from sequence to phenotype, to produce accurate predictions. This will include carrying out full molecular characterization within various biological communities with the ability to track spatio-temporal dynamics and predict emergent properties. Developing this broad capability will be focused in the near term on enhanced understanding of the novel coronavirus SARS-CoV-2 and the development of effective mitigation options for COVID-19.

ROLES OF DOE LABS AND THEIR PARTNERS

DOE's team-science heritage and systems approach to application-focused science and technology has proven decisive in pursuing critical S&T opportunities; its next advancements will use collaborative, multidisciplinary work to fully address 21st Century biology. To achieve these goals, DOE-supported investigators will carry out work in a range of areas building on current expertise. DOE's strengths in high-performance computing, simulation, and artificial intelligence can be utilized to handle enormous data streams with multi-omic information that is dynamic in space and time. Approaches to gather, curate, and store data are an integral part of enabling sophisticated data analytics. Visualization tools, data integration, security, and "privacy-observant" approaches will be required for these data. There also will be a need for multi-modal, quantitative, high-throughput observational technologies that are both automated and autonomous and driven by artificial intelligence. Molecular dynamics and multi-scale materials model approaches will need to be expanded to produce complex and high-resolution models. And, of course, the complexity of the problem and the importance of the applications mean that formal uncertainty quantification will be required.

DOE researchers are already involved in many of the converging technologies that will be key to realizing these benefits. They include:

- *Engineering DNA*. Tools to enable the production of chromosomal DNA and the engineering of entire genomes.
- *Biomolecular Engineering.* The engineering of functional macromolecules, the design of complex circuits and pathways, and regulatory system dynamics.
- *Host Engineering.* The engineering of cell-free systems, host cells and organisms, communities, and their integration and interaction.
- *Biosystems Design.* The application of the full capabilities of data science and artificial intelligence to develop a more rapid and agile methodology to design complex biological systems.
- *Bio-manufacturing.* The tailoring and fabrication of model biological systems, the creation of bio-compatible sensors, and advanced and economic production of bio-derived products.

Current DOE mission responsibilities and ongoing research and development efforts are in place and ready to pursue these critical research questions:

- The National Virtual Biotechnology Laboratory is a consortium of the department's 17 National Laboratories initiated in March 2020 to respond to the pandemic. It serves as a clearinghouse for access to experts and equipment across the entire lab system and is executing a collaborative research and response program targeting COVID-19.
- The Office of Biological and Environmental Research has the leading federal program in biological research underpinning the production of biofuels and bioproducts from renewable biomass, including in the related areas of genomic science and engineering and microbiome data science.
- The Bioenergy Technologies Office has the leading federal program in the conversion and scale-up of sustainable biomass resources into useful biofuels, bioproducts, and biopower. It also has launched multi-laboratory initiatives to accelerate the translation of biomanufacturing technology to industry.
- DOE has decades of biodefense expertise and world-class capabilities in many of the relevant technological areas (chemistry, computational biology, materials science, high performance computing, modeling and simulation, and risk analysis). DOE also connects this scientific and engineering expertise to the defense and intelligence communities.
- DOE is prepared to bring its rapidly expanding capabilities in artificial intelligence to accelerate advances in biotechnology, biomanufacturing, and biodefense.

While the work of DOE and partner departments and agencies is important, the impact of strategic government investments in biotechnology is amplified by much larger investments in the private sector. The size of the expanding biotechnology industry in the U.S. is already estimated to be $112 billion, with the majority in human health technologies. It is estimated that the emerging industry of bio-based energy, fuels, and products could grow to displace up to about 10% of fossil energy consumption by 2030 and represent a $260 billion industry. All developed countries have adopted bioeconomy-related policy strategies in the past decade driven by the need to address the threats to key resources: climate, water, energy, and land. Although private investment is massive and will continue to grow, it will not be optimized for certain important national security and other objectives — and that is a critical role for the government and the DOE labs.

A key part of investigating these biotechnology challenges will be an openness to new models of engagement across agencies and between parts of the public and private sectors. This includes robust partnerships between DOE and its laboratories and other government departments and agencies as well as with private sector partners: for-profit and non-profit, domestic, and international. New models that take into account best practices of open innovation might include multi-party CRADAs, nonprofit foundation(s) established for the DOE and its laboratories, expanded use of 501c3 and public good entities for partnerships, new approaches to joint workspaces, and others. Key agency partners will be HHS, VA, DoD, DHS, and Agriculture at the federal level. State and regional organizations may also be partners. The medical community, the agricultural community, foundations, industry, and non-governmental organizations are all stakeholders in the expanding bioeconomy.

In pursuing this S&T opportunity, DOE should open the activities to all its laboratories, encouraging collaboration and strong teamwork. DOE also should structure the work to address basic research questions, applied and systems work, as well as development and prototypes aimed at transition and deployment of technologies and tools.

II. Future of Accelerator Science, Technology, and Engineering

STATEMENT OF THE OPPORTUNITY

For nearly a century, accelerators have played a major role in the development of physical sciences, medicine, and industry around the world. Today, the DOE mission in discovery science and national security/nuclear stockpile stewardship depends critically on advances in accelerator science, technology, and engineering for mission success. DOE is recognized as the steward of this crucial area of science and technology, an important and far-reaching role due to the large and growing impact of accelerator applications across multiple federal agencies, as well as in health and medicine, energy security, industrial processing, advanced manufacturing, small-scale scientific research, border protection, and integrity of the electronics supply chain. Accelerator technology saves lives every day, impacts billions of dollars of commercial goods annually, and is vital to U.S. national security. This impact is propelled by advances in accelerator technology necessary to execute the DOE mission.

The mission landscape is evolving, resulting in new and proposed facilities across DOE programs that are anticipated to be significantly larger and more expensive than before. Confronting the most exciting and urgent scientific and societal challenges in the coming decades will require new instruments and facilities that push the limits of accelerator, material, detection, and computing capabilities well beyond those available today.

Over the next 10-30 years, the DOE Office of Science and NNSA will want to build major accelerator-based research and test facilities in the multibillion-dollar class, with particle colliders approaching the $10–30 billion scale if based on current technology. The size, complexity, and cost of these facilities demand new technologies and concepts to deliver a leap in performance while controlling size and cost. At the same time a new paradigm for success including international partnerships is needed. In the U.S., Fermilab is hosting an international program in neutrino physics (LBNF/DUNE) that includes the development of high-power proton beams (PIP-II) using the latest superconducting radiofrequency technology. The recently approved Electron Ion Collider, to be hosted by BNL in partnership with Jefferson Lab, is driving accelerator technology forward. The EIC will be the lead nuclear physics facility in the world for the next several decades and is expected to benefit from significant international contributions. In Germany, the nuclear physics Facility for Antiproton and Ion Research (FAIR) is using an international model for construction and operation. CERN along with European and U.S. partnerships is considering a 100-km circumference high-energy proton accelerator. The International Linear Collider (ILC), now being reviewed by the Japanese government as the potential host for the $5–10 billion facility, benefits greatly from technology developed at DOE labs, such as Jefferson Lab, SLAC, BNL, Argonne, LBNL, and Fermilab. The technology for these international efforts often depends on technology developed in DOE labs and U.S. industry. New tools for condensed-matter, material, chemical, and biological sciences research are primarily being built as multi-country efforts in Europe and international user facilities in the U.S. Another major international effort, ITER, not only shares multiple technologies with the accelerator field but ultimately relies on a high-power deuteron accelerator for materials testing (IFMIF).

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DOE, as the steward of these essential scientific and technical capabilities and infrastructure, needs to develop an aggressive and coherent strategy coordinated across the agency to advance critical technologies to assure U.S. scientific and technical leadership in the face of intense competition from around the world. These cross-cutting technologies provide the technical foundation for the scientific instruments of the future that will revolutionize our understanding of, and ability to engineer, material and biological systems, to explore the fundamental structure of matter, and enable wide-ranging applications in national security, fusion energy, next-generation nuclear medicine and industrial systems.

The U.S. needs to strategically determine when and how to engage in international partnership. While strategic reasons to construct domestic facilities without partners exist, such as with X-ray light sources and neutron sources, international partnerships tap into technologies developed abroad that might reduce the domestic development cost. It is strongly in the interest of the country to develop and own critical technologies that will have the largest impact. In this case, the U.S. would play leadership roles in the scientific program and benefit from the potential spin-off. Major technological advances are critical for meeting the national security mission and addressing the host of pressing applications described above, ranging from medicine to manufacturing to small-scale research.

The U.S. core capability in accelerator science and technology advances is not developing its full potential. We are building new accelerators at a fraction of the pace we did in the past, and they generally are based on decades old, mature technology that has been finely tuned and optimized. Game-changing accelerator innovation is exceedingly slow or completely absent. High-risk/high reward research in accelerator science is rapidly disappearing, having been replaced by an emphasis on sure bets from incremental improvements. This trend has led to diminishing technical expertise from an aging workforce and reduced talent pipeline, as well as aging technical infrastructure that in some cases is a half century old or more. The talent pipeline is a particular concern since many universities are not maintaining accelerator science and engineering curricula. This is at odds with technical challenges that are difficult and require the best and brightest to find solutions. The field must be vibrant and dynamic to serve as a magnet to talented young scientists.

The national lab accelerator-science infrastructure and the associated intellectual capital are in decline. For mass production, in some cases the technology has been transferred to industry. Yet many of these industries also are in decline for several decades as the demand for such devices has dropped in parallel with the declining number of accelerators built. This lab-industry partnership worked well in the past as the U.S. industrial complex has not had the R&D capabilities to innovate new, risky accelerator concepts; however, we now find the labs' and the U.S. industrial capabilities in a state of long-term decline with strategic implications for the nation.

The DOE Office of Science has initiated a complex-wide approach to accelerator science and technology. Adopting this approach is an important first step. Looking to the future, the U.S. must reevaluate its individual programs and procedures, and reinvest in this key field, even in times of tight budgets. Innovative science and engineering must be brought to the forefront to develop technologies that can drive down the size, cost, and complexity of new facilities while increasing performance. These new technologies will inevitably feed into accelerator applications at both the small and large scale, and lead to commercial spin-offs putting U.S. industry competitive in the global marketplace.

Specifically, critical technologies should be identified and aggressively advanced by setting clear goals and roadmaps, supporting the necessary fundamental science, and further developing capabilities and infrastructure to enable rapid development. Particularly critical technologies include particle acceleration, high-gradient acceleration, foundational materials science, high-field magnets, lasers, particle detectors and sensors, and optical systems. Promising directions, particularly those that are high-risk/high reward, should be rapidly brought to the demonstration phase.

Investments should be identified in the following key areas:

- Revitalize the accelerator science and technology infrastructure in our laboratories that enables a forefront national R&D program.
- Develop critical technologies the U.S. should "own" to secure a strategic technological and/or economic advantage.
- Develop demonstration projects with high potential on the scale of $10–100 million to assess new ideas at a rapid pace, allowing for significant progress to be achieved on significantly shorter timescales.
- Establish a vibrant talent pipeline for the next several decades with laboratories and universities working together.

ROLES OF DOE LABS AND THEIR PARTNERS

In the U.S., accelerators are being constructed at national labs for basic and applied science as well as national security. Plans are developed for new projects that extend for several decades based on accelerator technologies that exist today or are expected with incremental future developments. The national labs have the infrastructure and capabilities to carry out these large-scale accelerator projects and have the tradition of developing forefront user facilities that benefit researchers at national labs, universities, and industry.

This infrastructure has been used to develop prototype devices and first-article components for new accelerators. The labs understand high-risk/high-payoff research and how to translate R&D into solutions for real-world problems. The national labs are the obvious places in the U.S. to innovate, build, and operate large scale facilities and address the smaller scale high-impact applications. Due to the breadth and depth of multidisciplinary capabilities and the ability to mount teams to attack difficult technical challenges, the national labs are the best place to execute the research and development that will bring new ideas into practical use. National labs have extensive industrial and university partners, and as a result are in the best position to integrate the fundamental developments in the field while building the industrial base.

Investment in these key areas will create the advanced technologies and workforce to build the forefront, affordable facilities of the future, as well as the host of new and emerging applications across a broad front. The long-term vitality of accelerator science in the U.S. will be assured, making the nation a leader in this internationally competitive arena.

III. The Future of Deterrence

STATEMENT OF THE OPPORTUNITY

Since the end of the second world war, a key element of the defense strategy for the U.S. and its allies has been a robust nuclear deterrent constraining the actions of potential adversaries. The goal has been to deter aggression and convince adversaries they have more to lose than gain from attacks. In recent years, many considered nuclear deterrence a relic of the Cold War. But with the return to an era of great-power competition, the U.S. is pitted against an increasingly aligned China and Russia who are pursuing aggressive technology development oriented to economic and military objectives. They are our strategic adversaries, seeking to increase their global and regional influence while diminishing ours. U.S. restraint in avoiding new nuclear systems since the end of the Cold War has not been reciprocated. These countries also seek to undermine our democratic institutions. China is an increasingly capable economic and S&T competitor. In the increasingly great-power competitive landscape, investments in S&T are tools of nation-states that can be aligned to specific objectives and provide decisive advantages. Particularly in the case of China, there is a willingness to align across military, civilian, governmental, academic, and industrial participants. This renewed nation-state investment makes U.S. investment in S&T increasingly important.

The current geopolitical reality is more complex than that of the past 75 years with threats that are varied in potential adversaries and technologies. There continue to be asymmetric threats as well as non-military ones. Some threats, such as cyber or efforts aimed at manipulating democratic processes, are difficult to attribute and may not trigger an armed response. Uncertainties in the future security environment are compounded by the risk of disruptive technologies — from hypersonics to engineered biothreats to quantum information technologies — and are steadily increasing as the technical sophistication of our strategic adversaries (notably China) increases. In addition to ensuring the effectiveness of the nuclear deterrent, the U.S. must ensure deterrence aimed at emerging threats (such as that posed by contested earth orbit), the ability to attribute the origin of an attack, increasing the resilience of our vital infrastructure systems, and the development of future, non-nuclear or non-military deterrence options. Because of this an even broader set of S&T areas needs leadership from DOE.

Taken together these trends point to a need to evaluate how nuclear deterrence and approaches that might complement it should evolve. It will be necessary to respond to evolving threats and countermeasures with systems that may move beyond life extensions and have implications for the science and technology underpinning the certification of the stockpile in the absence of nuclear testing. We must transition from maintaining the existing stockpile to creating a responsive, agile, cost-effective design and production capability for the stockpile of the future.

Deterrence continues to be enabled by forces-in-being such as the nuclear stockpile designed by DOE's NNSA coupled with military delivery systems and the entire DoD enterprise and by latent and responsive capabilities. Leadership in the most advanced S&T in support of the deterrent has been critical since the discovery and application of nuclear physics to national defense. Going forward, DOE must more explicitly address the dual use implications of new technologies in a manner that engages the entire department, especially NNSA and the Office of Science, and ensures high quality S&T for nuclear responsiveness in the NNSA — for advanced manufacturing, science for surveillance, complexity and uncertainty analysis, and analysis alerting the U.S. to over-the-horizon technical threats.

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The future of the United States as we know it depends on this. We must be able to deter destructive military and other attacks and protect our critical infrastructures (such as energy, finance, and internet). Providing a scientific and technological capability that supports our national security has been a mission driver for DOE and its predecessors since creation of the national labs following the second world war. While stockpile stewardship has proven an effective means of ensuring the safety, security, and reliability of the current Cold War-era deterrent since the end of underground testing, changes in the global environment require an evaluation of what will be needed going forward. This is made more challenging by the fact that the United States no longer has assured scientific and technological leadership with the attendant risks of surprise and potential economic consequences of loss of dominance in areas of future technology disruption.

The threats due to advanced technologies (e.g., internet, new materials, lasers, photonics, GPS, and nano-electronics) are so broad that the capabilities of all 17 DOE National Laboratories will be needed to stay abreast of and help counter all the potential dual-use technologies that may touch everyone's lives and underpin future U.S. economic competitiveness.

One of the roles of the labs is to provide the underlying science, forensic, and attribution capabilities needed to avoid technology surprise and support a flexible and reliable approach to future deterrence across a spectrum of threats and contingencies. The development and foundational understanding of novel high-performance materials and advanced processing technologies will be key. For the nuclear deterrent this includes a need to: understand and certify materials performance under extreme conditions; develop high-resolution *time dependent imaging of implosions* using appropriate geometries and materials; follow a path to *thermonuclear ignition* for boost physics and secondary physics; develop functional materials for advanced detection to ensure early warning, attack understanding, and rapid decision-making; and manufacture of world-leading radiation hard semiconductor materials. The continued advancement of modeling and simulation and the computing platforms that enable it will be essential for maintaining U.S. leadership in integrated, information-centric systems. At the same time, we must reassess how we support Discovery Science — fundamental far-reaching R&D that could lead to breakthrough technologies in areas such as bioengineering and quantum information.

Major technologies that may be likely to result in transformational technology surprise have been captured in the other four S&T opportunities outlined by the laboratory directors in: (1) Computing, (2) Applied Biology, (3) Accelerator Science and Technology, and (4) Energy Systems. Focusing on these areas will provide a venue to stay in touch with major technology developments worldwide that could become a threat (especially when we cannot be S&T leaders in every area). The national lab system is just the environment to nurture the needed innovations — from what goes on in the labs through university collaborations, and interactions with the community at the department's constellation of user facilities.

We urge the DOE to adopt a "one DOE" approach that cuts across the silos within the department to increase the focus on the interfaces between key disciplines that are perhaps most likely to be the source of future technology surprise. The research roadmaps laid out in the S&T opportunities can provide a guide to implementing this recommendation. These other four opportunities, together with broader applied energy and science efforts, support all aspects of deterrence by being the public part of DOE S&T excellence. Other programs, such as those in the NNSA, enable DOE to fully understand and assess the less public end of the dual-use spectrum. Collaborations between the labs and interaction between the practitioners of forefront S&T and national security will be essential.

ROLES OF DOE LABS AND THEIR PARTNERS

Partnerships must happen across the DOE enterprise, including with industry and academia. International engagements will be an imperative to ensure the United States takes advantage of key developments worldwide while protecting our most sensitive developments. These international engagements must be made in full knowledge of the real risks because the benefits, if done well, far outweigh them. Public/private partnerships, especially in areas such as energy and cyber, will also be important. Finally, the coordinated efforts of all 17 DOE National Laboratories will be essential in addressing the deterrence challenges that face the nation.

IV. The Future of Computing

STATEMENT OF THE OPPORTUNITY

DOE mission drivers across science, energy, and nuclear security have pushed innovation in computing since the earliest days of the national laboratory complex. Today the labs, working closely with industry, continuously push the farthest frontiers of computing, networking, and related technologies in support of scientific discovery. Many of those breakthroughs migrate from high-end science and engineering to commercial applications and eventually trickle down to everyday life.

During the past 30 years the growth of computing has been driven by advances in microprocessor performance based on Moore's Law. The next 30 years will see a dramatic change in computing technology and the characteristics of computing platforms will be substantially different from today. While some trends are visible today, it is not clear what the computing and networking landscape will look like 30 years from now. The DOE national labs have a long and distinguished history of advancing computing technology, architecture and platforms, software and algorithms, and application to address the most challenging problems in science and engineering. DOE's investment in advanced scientific computing has assured global U.S. leadership in the field. The changing international competition in S&T and the significant role computing plays for leadership in science, national security, and economic competitiveness make it essential that computing continues to be vigorously pursued.

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The computing opportunity is computing supremacy: developing and maintaining a superior world-leading computing ecosystem that addresses the most critical challenges in scientific discovery, energy assurance, economic competitiveness, and national security. This goal encompasses the development of an entire computing ecosystem: applications, algorithms, system software, hardware technologies and architectures, the networking and data infrastructure, along with critical workforce development. This is the current state of DOE exascale computing for modeling and simulation. It must be maintained and extended to include rapidly developing new technologies, described in the next section, while also addressing new challenges and opportunities arising from the rapidly growing availability of large-scale data and new tools for data management and analysis.

For the first part of the next decade exascale computing will be the primary activity. The exascale computing project (ECP) is a multi-lab effort focused on hardware and software and the associated machine deployments planned for the next level of systems leading up to exascale performance. In addition to high performance for the modeling and simulation that supports science, engineering and stockpile stewardship, the new generation of machines will offer exceptional capabilities for data analytics to deal with the large volumes of data arising from DOE experimental programs and facilities and generated globally from large sensor networks. These platforms will be ideal systems to explore the application of AI and machine learning in science and DOE mission applications. Development of future sensor networks for global situational awareness and risk management and response would be a natural complement to the AI capabilities of exascale class systems.

Toward the end of the 2020s CMOS technology might be coming close to its inherent practical limits given that the increasing time between successive generations of smaller transistors — the underlying enabler of Moore's Law — has signaled its approaching end. With it goes the economic free ride on the back of faster-cheaper information processing. Exascale represents a push to extend the power of conventional CMOS technology until the end of Moore's Law. For this reason, it is important to find ways to improve computational power free from such limitations. The national labs have an ideal knowledge base to explore digital computing technology beyond Moore's Law, leveraging investment in material science, materials characterization and fabrications facilities, light sources, and advanced manufacturing.

In this time frame computing technology will likely diverge according to application. The 2010s experienced such a specialization in the creation of GPUs, which were still universal processors. In the 2020s we will see the emergence of specialized processors for AI/ML, which are far more narrowly targeted. Private sector investments to develop specialized hardware have been used to great effect to accelerate AI/ML, smart-phones, autonomous vehicles, and soon 5G networks. Market forces will drive those investments to follow narrower threads of opportunity, targeting technologies that solve specific, non-universal computational problems. Mutual benefit will diminish. That splintered landscape threatens to undermine the broad-based economic growth and scientific advancement that has fostered U.S. global leadership for decades. Disruptions will reverberate from the economy to science to national security. In this era of extreme heterogeneity, the national labs will provide the necessary leadership to advance computing in an increasingly complex environment.

Current investments in quantum information science (QIS) will lead to the demonstration of quantum advantage in computing and simulation on scientific problems. Mature quantum computers in the 2030s will not supplant digital technology but complement it. Fundamental questions in QIS still need to be addressed, but it can be expected that quantum computing will reach a maturity in the next decade to become a useful tool for DOE mission applications. Beyond computing and simulation, quantum approaches show promise to provide new capabilities and tools for sensing and metrology, and communication. This is vital for fundamental research and promotes security, health, and the economy.

Developments in networking will parallel the advancement of computing technology. Wide area networking needs continuous development to support the growing system of exascale computers, large-scale scientific facilities, and experimental data gathered from distributed sensors. The trend of integrating computing and storage within the network for distributed edge computing, caching, and other science functions will greatly evolve the role of networks. 5G networks will deliver new capabilities for the DOE mission that still need to be fully explored. By the early 2030s an important threshold should be crossed: Broadband wireless networks beyond 5G and low-orbiting satellites (LEO) will have a greater bandwidth than what's available within computer systems. This crossover point will open a whole new era of wireless technology breakthroughs that we can't imagine today, just like we could not imagine a smart phone in 1990.

In addition to sustaining current efforts in exascale, quantum, and networking, three growth opportunities exist:

1. An ongoing effort to develop algorithms and applications that fully exploit the capabilities of conventional and future extremely heterogeneous architectures. In many cases software innovation has dramatic payback on already deployed systems and the scientific and security applications that support the DOE mission often do not cater directly to commercial markets in a way that would support the strategic investments that will need to be targeted narrowly based on specifics of the technology platform.
2. Development and deployment of intelligent sensors that, combined with data analytics, integrated edge computing capabilities, and high-performance computing, could transform our awareness and understanding of the physical world around us.
3. Development of cybersecurity systems and approaches that protect not only the computing infrastructure that will be developed, but the digital and physical infrastructure of the nation.

ROLES OF DOE LABS AND THEIR PARTNERS

It is difficult to envision the range of computing technology and applications in 2050, but it can be said that the national labs will be able to address the challenges because of close collaboration among physical, computational, and earth and bio scientists, mathematicians, and engineers. The labs have demonstrated an enterprise-wide multidisciplinary approach that has driven co-design and the exascale computing project. This approach can be applied to software and sensor efforts, and it will magnify the impact in the foundational developments of exascale and quantum.

Computing is fundamental to all the other opportunities — accelerator design, biology, deterrence, and energy. None of these topics can progress without computing. We don't know today what the computing challenges in the other disciplines will be, so we must build the skill set and infrastructure of future computing to be prepared to solve them. Without computing, all the other S&T opportunities will be at risk. The broad DOE lab mission requires a deep competency in computing and networking with highly qualified staff able to innovate with the mission science collaborations that rely on computing for success. Future science breakthroughs will depend on computing — it accelerates scientific discovery. Lastly, continued investment in computing is needed to avoid technology surprise by our adversaries. The computing industry accounts for a $1.8 trillion contribution to the U.S. economy and 11.8 million jobs. The national labs have made and will continue to make a major contribution to maintaining the competitiveness of this industry by being at the leading edge of exploring computing, understanding technology developments, and developing new applications for challenging science and engineering problems.

Successfully addressing this challenge will take robust partnerships between DOE and its laboratories and other government departments and agencies along with private sector partners including for-profit and non-profit, domestic and international. An openness to new models of engagement across agencies and between the public and private sectors will be needed. New models of open innovation might include multi-party CRADAs, a DOE and/or laboratory foundation(s), expanded use of 501c3 and public good entities for partnerships, new approaches to joint workspaces, and others. Key agency partners will likely be DoD, NASA, HHS, VA, NSF, and DHS, at the federal level. State and regional organizations also might be partners. Foundations, industry, and non-governmental organizations will be partners on the private side.

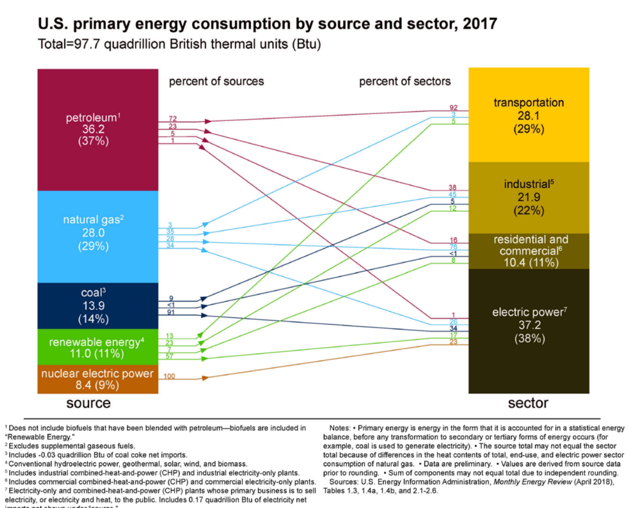
DOE should open the activity on the S&T opportunities to all its laboratories, encouraging collaboration and strong teaming, and structure the work to address basic research questions, applied and systems work, and development and prototypes aimed at transition and deployment of technologies and tools.

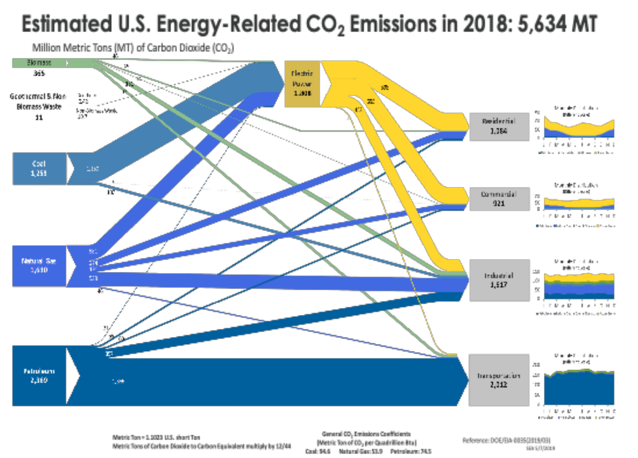
V. The Future of Energy Systems: Innovating a pathway to the Future of Energy Systems

STATEMENT OF THE OPPORTUNITY

We face increasing challenges for energy services on a planet where by 2050 the world population is projected to increase by 30%, the global GDP will double, and global energy consumption is anticipated to increase by 50%. In the absence of significant changes to the current energy system — and especially to the current mix of power generation sources, distribution and usage, transportation fuels, and absent the development of effective mitigation strategies for carbon emissions — CO2 emissions are projected to lead to a highly consequential global temperature rise beyond 2°C. While energy intensity continues to decrease, as it has for decades, it will be insufficient to ameliorate this consequence.

The current energy system is incapable of addressing these challenges. Significant advances in science and technology must enable a flexible energy system of the future, providing power and fuels originating from a variety of sources in a seamless manner, including natural gas, coal, oil, nuclear (fission and fusion), hydro, bioenergy, solar PV, concentrated solar, wind (onshore and offshore), geothermal and marine energy. Today, about 80% of the total world energy consumption is met by fossil fuels. Non-hydro renewable energy sources (geothermal solar, wind, and biofuels) contribute about 3% of energy, another 11–12% is provided by biomass waste and hydroelectric power, and the remaining 5% is from nuclear. A S&T opportunity for the U.S. and the world is to develop appropriate pathways, strategies and plans for a future energy system to meet the growing demand for energy, from homeowners to commercial entities to industrial manufacturers, while also decarbonizing energy production to net-zero carbon emissions by 2050 (and net-negative carbon emissions in the second half of this century). It must, moreover, facilitate economic prosperity, and it must be secure and resilient.





FUTURE STATE

Electric power, industrial, residential and commercial, and transportation are the primary elements of the nation's energy system (see illustration for source-to-use mapping and associated carbon emissions). While today 80% of the energy is supplied from fossil sources, in the future (2050), the fossil fuel contribution will be much lower, and will likely include carbon capture storage and utilization (CCS), wherein CO2, via a range of processes that will likely involve electrocatalytic and biological approaches, together with cheap electrons, is converted to chemicals, fuels and materials. The goals for the endpoints of the system elements are reasonably understood, but the pathway to achieve them is not; they are dependent on several scenarios, influenced by technological developments, policies, economics, and locally available resources.

As we move toward the future state, the energy system must evolve to a low-carbon state, and to do so requires a higher reliance on clean fuel systems and electricity. While the precise 'system of the future' remains to be determined, it will include, in some combination, renewable energy sources, advanced nuclear (potentially including fusion as well as fission) and fossil fuels incorporating large-scale CCS. To state it simply: We need to wean transportation from oil, evolve the residential/commercial sector (power and fuel) from fossil (coal, oil, natural gas, without CCS) to clean sources, and move electric power generation into renewables and nuclear, eliminating the current non-CCS use of coal and natural gas. The trick is to do all this on the fly while maintaining delivery, resilience, and security, without disruption of the economy or the nation's standard of living.

The energy system of the future will be significantly more versatile and operate autonomously, using artificial intelligence and machine learning. Beyond two-way power flow, which already occurs, it will efficiently manage tens of millions of energy resources (DER)s, including roof-top solar, sensors, EVs, distributed wind energy, and energy storage, including behind-the-meter storage. Energy storage over time scales from a few hours (batteries) and pumped hydropower to seasonal (utilizing chemical bonds) will become a key part of the new energy system. By 2050, battery power will be safe, and the cost of storage will be sufficiently cheap, such that EVs will likely be cheaper than internal combustion vehicles (the goal is by 2023). This will accommodate the integration of significant amounts of variable renewable (wind and solar) resources. The transportation sector would benefit from power from the new system. This will include not only production of electricity, but for H2 generation (expected to largely be for heavy duty trucking), synthetic methane and a range of fuels, including biofuels, all of which will rely on carbon capture and utilization and power derived from cheap renewables, or other cheap sources, potentially nuclear or geothermal. The buildings of the future will be grid interactive, thereby optimizing energy use; they will no longer operate as static loads. Power electronics interfaces, connecting VREs pumped hydro and heat sources, will be ubiquitous and the grid will transform to become inverter-based, which will be more efficient than the current synchronous power generation grid. Baseload power (nuclear, geothermal) is still important and will contribute to flexibility of the grid. This transformed, flexible grid interconnected across the entire nation could effectively take advantage of resources (wind, solar, geothermal, nuclear) that vary geographically.

The concept of integrated energy systems (IES), in which a variety of energy sources, both electrical and thermal, contribute to produce flexible energy for manufacturing, clean water, chemicals, and the electric grid — important for the low-carbon energy future — will become a reality. The National Laboratories are currently developing roadmaps necessary for this transformation.

While the current, intermediate, and desired final states of the future energy system may be relatively clear, the pathway to achieving these goals given constraints on the evolving system remains murky. Energy systems of the future must be resilient (i.e., maintain a degree of operation in the midst of cyberattacks and disasters) and cost effective. There is a complex interplay between privately owned resources and the need for a reimagined, coordinated electric grid with significant coupling to the transportation and industrial sectors. Addressing this opportunity involves understanding the complex interplay between advances in science and innovation, technology development, markets and economics, capital investments, infrastructure, policy, and political factors.

Determining pathways to the future energy system is an enormous systems-engineering problem. Systems engineering principles combined with advances in artificial intelligence/machine learning (AI/ML) provide the key to developing a new analysis framework. Flexibility for accommodating major unexpected technological innovations, such as occurred with hydraulic fracturing and horizontal drilling to enable shale gas production, must be built into the system.

The National Laboratories are well equipped to develop a revolutionary AI/ML-based framework for analyzing energy systems pathways, drawing from world-class capabilities in systems engineering, domain expertise in all aspects of energy generation and use, and techno-economic analysis, and combining it with data analytics, advanced AI/ML algorithms and analysis, and 'big iron' computing horsepower. The first step is to develop a conceptual design of a system framework that would use AI/ML to analyze multitudes of energy system options in the presence of market conditions. A wide variety of published energy system scenarios are available as input for the options. The labs will build the framework for "debate on a computer" that will allow various pathways to compete, through algorithms, for optimized energy system outcomes.

An even greater challenge is moving from the identification of potential pathways to detailed blueprints of the needed energy system transformation. The application of AI/ML concepts must be combined with subject-matter expertise to develop plans for and execute at-scale demonstrations of the computational energy system pathways.
These technical results will form the basis for policy implementation that will drive the system transformation. The laboratories will, therefore, act as architects to turn concepts into concrete plans for the energy system of 2050.

ROLES OF DOE LABS AND THEIR PARTNERS

The Energy Systems opportunity is of sufficient magnitude that no one industry can solve it; government investments will continue to be necessary. The 17 DOE laboratories possess huge capabilities in the advancement of technologies across the full spectrum of energy sources, ranging from fossil fuels to renewables, combustion to batteries, chemicals to biomanufacturing. Further, the laboratories represent the nation's premier set of research facilities, including world-leading computing capability and associated computer science expertise, light and particle sources, and nanoscience centers. The applied energy lab R&D facilities include source-specific capabilities (renewables, fossil, nuclear) and also energy system integration facilities at a wide variety of scales. The DOE National Laboratory system is already playing lead roles in several areas: the Grid Modernization Initiative, next-generation batteries for grid storage and electric vehicle technologies, integrated/hybrid energy systems, and carbon capture and utilization technologies.

The laboratories collectively have the broadest expertise across the full portfolio of energy resource options as well as the deep technical and economic expertise needed to adequately assess future energy system pathways considering the constraints of this evolving system including deployment inertia, technical advances, economics, policy environments, and system dynamics. To meet this opportunity the labs will need to partner closely with industry and universities, with the DOE playing a convening role, to analyze the technical and economic feasibility of a full ensemble of energy system pathways that lead to deep decarbonization of the full energy system across the electricity, transportation, industrial, residential, and commercial sectors. The labs will collaborate with academia on early stage foundational research and with industry on later stage research and validation. These analyses will require an integration of several DOE, lab, and private-sector energy deployment models as well as development of a common set of model details, resolution, and system granularity to enable full energy system integration to adequately assess the opportunities and impacts of system changes.

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