SCIENCE TO ACCELERATE SOLUTIONS TO U.S. ENERGY, CLIMATE, AND ENVIRONMENTAL EQUITY CHALLENGES

NATIONAL LABORATORY DIRECTORS' COUNCIL

JANUARY 2021

The existential threat of climate change requires swift, bold, and strategic action. Although progress has been made to date, the current best understanding of climate science and today's most advanced clean energy tools and technologies are inadequate. To truly change our trajectory and meet the Biden Administration's ambitious climate, energy and equity goals will require the transformational change that comes from fundamental scientific discovery. The Department of Energy's 17 National Laboratories, with their world-class expertise, facilities, and research programs, can help deliver the fundamental science breakthroughs that will drive solutions at the scales required to move the world toward a more sustainable and equitable future.

As described in a companion paper *Fundamental Science: Critical to Meeting U.S. Energy and Climate Mitigation Goals*, the DOE should immediately leverage and strengthen its existing climate, energy, bioscience, and environmental research programs and capabilities. This paper describes four specific, illustrative examples of how DOE can pursue use-inspired fundamental science breakthroughs in support of its climate and clean energy goals. In addition to renewed attention to and better leveraging of existing programs, the initiatives below will further build on the national laboratories capabilities to deliver solutions at the scales needed.

Advance Energy Storage Technologies. New forms of energy storage will be critical to decarbonizing the economy and transforming our energy system into the integrated, flexible, and resilient one we need for the future. Achieving these goals requires an investment in fundamental chemistry and materials science; high-risk, high-reward technology concepts; and close coupling of fundamental science and early-stage technology development. DOE's National Laboratories have the leading expertise; a successful track record leveraging collaborative, team-based multidisciplinary approaches; and unique light- and neutron-sources, computing, nanoscale science, and data facilities needed to deliver on this challenge.

Accelerate Discovery of Net-Zero Materials, Chemicals, and Manufacturing Processes. There are many parts of our economy that contribute significant emissions, but do not lend themselves to electrification. To achieve a resilient, equitable, and affordable net-zero emissions economy, new materials, chemicals, and manufacturing processes are required, as are efforts to research, develop, demonstrate, and deploy them as candidate technologies at unprecedented scale. A broad cross-complex investment that integrates DOE's core fundamental science programs and expands access to its User Facilities is needed to accelerate an economy-wide transition to net-zero technologies.

Advance Human-Earth Systems Models to Support Science-Based Decision Making. Addressing climate and energy challenges in an equitable way requires deep technical analyses and assessments built on a foundation of strong fundamental science across a wide range of disciplines. While integrated human-Earth system models currently provide valuable insights, fundamental science challenges remain in understanding integrated human-Earth systems, both in how models are constructed to provide valuable insight and how they are used for multisectoral decision-making. Addressing these challenges requires new investments in human-Earth system observations and modeling capabilities that focus on human-Earth system predictability at decision-relevant physical and time scales.

Advance Negative Emissions Technology & Science. Addressing the climate crisis requires the large-scale deployment of many negative emissions technologies. However, there remain fundamental science challenges that must be addressed to fully realize the potential of these technologies. The National Laboratories steward world leading research programs and capabilities that can directly address the discovery science required to meet these challenges. From research into the sustainable modification of soils, plants, and their interactions to enhance natural carbon sinks, to utilizing carbon in biofuels and advanced bioproducts, the DOE National Laboratories are already studying how to effectively capture, store, and convert carbon emissions into multiple desirable outputs that can bolster the growth of the US bioeconomy. Additional investments and strategic alignment of programs would speed the delivery of economically viable and sustainable approaches for capturing and converting CO_2 at the scale required to meet emissions reduction goals.

We recommend DOE convene a series of Department-wide roundtables and workshops in FY 2021 to set priorities, ensure cross-agency coordination and cooperation, and inform the scale and scope of investments necessary to achieve the Biden Administration's goals and objectives. The Department has a wide range of funding mechanisms that can be used to assemble a strategic portfolio of investments starting in FY 2022 that can most effectively leverage the expertise and facilities of the National Laboratory complex, as well as the academic research community, other state and federal agencies, and the private sector. By clearly communicating high-level goals and priorities, the Department can galvanize the broad research community around common objectives and thereby accelerate the pace of clean energy and climate innovation, bolster U.S. economic competitiveness, and reassert our global leadership in science and technology.

Each of the four illustrative examples is described in more technical detail below.

I. Advance Energy Storage Technologies

The climate emergency requires new forms of energy storage to decarbonize the economy and transform today's diverse energy sources and uses into an integrated, interactive, resilient, and flexible energy system. Achieving these goals requires high-risk, high-reward research and close coupling of basic science and early-stage technology development, of the type only possible at DOE's National Laboratories with their leading expertise; collaborative, team-based multidisciplinary approach; and unique facilities spanning light- and neutron-sources, computing, nanoscale science, and data management.

Today's Li-ion batteries have the potential to decarbonize personal and light-duty transportation. Combined with wind and solar generation, they may be able to decarbonize up to 50 – 60% of the electricity grid[1] (Albertus 2020). However, the cost, safety, recharge time, energy density and lifetime of Li-ion batteries prevent them from decarbonizing heavy-duty transportation (including long-haul trucking, rail, maritime shipping, and transcontinental aviation) and economically stabilizing the grid for more than 4 – 6 hours. Pumped-storage hydropower, the dominant form of grid storage today, can stabilize the grid for longer times, typically up to 20 hours, though consecutive days of stabilization are needed for overcast or calm weather. Further, much of heavy industry, including the manufacture of steel, cement, and high-value chemicals, relies on large quantities of high-temperature heat supplied by combustion of fossil fuels. A low-carbon replacement for high-temperature heat from fossil fuel combustion is a critical need for decarbonizing the U.S. economy.

There are rich, ripe opportunities for **next-generation electrochemical, chemical, and thermal energy storage** to meet these climate emergency needs. For instance, high-energy-density metal-air (Zn, Li, Na), multivalent (Mg^{++}, Ca^{++}, Zn^{++}), and conversion cathode (Li-S) batteries extend heavy-duty electric transportation to regional scale[2]. Chemical storage in hydrogen and low-carbon liquid fuels (ammonia, green hydrocarbons) can decarbonize heavy-duty transportation at continental scales[3]. Long-duration aqueous/organic flow batteries[4] can stabilize the electricity grid for days at a time. Combustion of chemical storage media such as hydrogen, its low-carbon fuel derivatives, or solar fuels can provide the high-temperature heat needed to decarbonize heavy industry[5], as well as provide seasonal storage for the grid and combustion heat for buildings. Finally, subsurface thermal energy storage in underground rocks and aquifers and molten salts and phase-change materials can provide seasonal storage[6] and capture solar and nuclear heat for residential, commercial, and industrial use.

Advances in all storage technologies, including solar fuels, batteries, hydrogen, low-carbon liquid fuels, and thermal, require the utilization of the major User Facilities, including light and neutron sources, high-performance computing, and nanoscale science centers at DOE National Laboratories. These facilities are essential to pioneering the **development of new catalysts to speed up chemical reactions, new materials for anodes, cathodes and electrolytes for batteries, solar fuels conversion, electrolyzers and fuel cells, and thermal storage materials for thermal storage media** with high heat capacity and latent heat. These facilities, spearheaded

1 Albertus et al., "Long-Duration Electricity Storage Applications, Economics, and Technologies." *Joule* 4, 21 (2020).
2 Trahey et al., "Energy Storage Emerging: A Perspective from the Joint Center for Energy Storage Research." *PNAS* 117, 12550 (2020); Forrest et al, "Estimating the Technical Feasibility of Fuel Cell and Battery Electric Vehicles for the Medium and Heavy Duty Sectors in California." *Applied Energy* 276, 115439 (2020)
3 Staffell et al., "The Role of Hydrogen and Fuel Cells in the Global Energy System." *Energy Environ. Sci.* 12, 463 (2019).
4 Li et al., "Recent Advancements in Rational Design of Nonaqueous Organic Redox Flow Batteries." *Sustainable Energy Fuels* 4, 4370 (2020).
5 Friedmann et al., *"Low-Carbon Heat Solutions for Heavy Industry Sources, Options, and Costs Today."* Columbia CGEP Report, 10-7-19.
6 Carlsson. "Coarse-Grained Model of Underground Thermal Energy Storage Applied to Efficiency Optimization." *Energies* 13, 1918 (2020).

by DOE at the National Laboratories, provide an atomic perspective of materials and phenomena and enable inverse design at the atomic and molecular level of energy storage materials and systems.

Discovery of new materials and chemistries and scaling them to commercial levels will require significant concerted back-and-forth interaction between basic and applied scientists, drawing on expertise, facilities, and a research environment only available at National Laboratories. The emerging **science of inverse design using artificial intelligence enabled by high-performance computing and one-of-a-kind materials databases** will rapidly accelerate the pace of materials discovery, opening new and untapped design spaces for energy storage.[7] Developing these inverse design algorithms and coupling them to robotic synthesis and characterization at light sources and nanoscale science centers in **self-driving materials discovery laboratories** is a powerful and potentially transformative opportunity for fundamental science and commercial development. Accelerated discovery of new materials and rapid maturation to commercial viability is critical to meet the ambitious 2015 Paris targets of 50% decarbonization by 2030 and 100% by 2050.

New energy storage paradigms offer much more than decarbonization opportunities — they integrate separate energy sectors into a single unified, interactive, flexible, and robust energy system. Electric vehicles (EVs) are a prime example, uniting previously separate transportation and electricity technologies; decarbonizing both with wind and solar electricity; and enabling digital monitoring and control of vehicle location, speed, route, and charging schedule while easing traffic congestion. As EVs proliferate, the energy stored in their batteries is an enormous resource that could stabilize the grid or supply local needs in emergencies, such as extreme weather or intentional outages due to wildfire risk in California. Hydrogen and electricity as complementary energy carriers are a second prime example, with full interchangeability between the two through electrolyzers, fuel cells, and hydrogen combustion turbines. Electricity and hydrogen can both decarbonize transportation, with batteries powering light-duty personal cars and urban delivery vehicles, while hydrogen powers heavy-duty applications such as long-haul trucks, rail, shipping, and transcontinental aviation. Combustion of hydrogen or its derivative fuels can decarbonize heavy industry, an application that electricity cannot easily serve. This integration of previously separate energy sectors opens new horizons for flexibility, resilience, and innovation in the energy system.

Fundamental science at National Laboratories is central to discovering and developing the new materials, chemistries, and low-carbon fuels required for fully decarbonizing long-haul transportation, the electricity grid, and heavy industry. Unique User Facilities enable direct observation and simulation of materials at atomic and molecular levels, a critical feature of new materials discovery. These new energy storage discoveries must then advance from the laboratory to technology development through close cooperation with applied technology programs such as the Vehicle Technologies, Hydrogen and Fuel Cells, Building Technologies, and Advanced Manufacturing Offices in DOE EERE; the Technology Development Office and Grid Storage Launchpad in DOE's Office of Electricity; and the Energy Storage Grand Challenge. New high-performance materials are urgently needed for **anodes, cathodes, and electrolytes for batteries, electrolyzers and fuel cells; catalysts for production of low-carbon fuels (e.g., ammonia and green hydrocarbons from H_2, CO_2, and N_2); low-cost, durable materials for hydrogen pipeline networks; and thermal storage materials with high latent heat and heat capacity and with thermal conductivity** designed for the application. In addition, many current and proposed energy storage approaches require critical minerals that have become increasingly scarce. Expansion of domestic use will require entirely **new energy-efficient and sustainable approaches to separations and purification of critical minerals** from mineral compounds and solutions, an all-of-DOE effort at the intersection of geology, geochemistry, materials science, chemical engineering, and environmental science.

7 Crabtree. "Self-Driving Laboratories Coming of Age." *Joule* 4, 2538 (2020).

II. Accelerate the Discovery of Net-Zero Materials, Chemicals, and Manufacturing Processes

Transitioning to a net-zero emissions economy will require decarbonized electrical power, an integrated grid, electrification where possible, clean fuels for the parts of the economy that are not easily electrified, alternative construction materials and manufacturing processes for them, and new approaches to removing and recycling carbon from the atmosphere. **To achieve robust, reliable, equitable, and affordable net-zero emissions in energy, industrial, and agricultural systems, new materials, new chemicals, and manufacturing processes are required, as are efforts to research, develop, demonstrate, and deploy them as candidate technologies at unprecedented scale.** The creation of Hub-scale networks connecting and expanding DOE-wide expertise, facilities, databases, and capabilities to enable the emerging science of inverse design of materials — whereby a material is developed to exhibit one or more predefined properties — and using artificial intelligence, coupled with tailored high-performance computing facilities and one-of-a-kind materials databases, can rapidly accelerate the pace of materials discovery, opening enormous design spaces for bringing these critical processes and pathways to market. In this way, the National Laboratories' expertise and unique capabilities in fundamental materials science and chemistry will play an essential role in accelerating the decarbonization of "hard-to-decarbonize" sectors.

Just as there would be no semiconductor industry without basic science, **fundamental discoveries of new materials and chemical processes, and an interplay between these discoveries and technology development, will be foundational for the creation of net-zero U.S. energy and industrial sectors,** addressing not only emissions, but also equity and justice for historically impacted disadvantaged communities across the country. The DOE National Laboratories have pioneered transformational capabilities and large-scale facilities that have allowed us to understand and control matter and energy in unprecedented ways. These include, for example, the harnessing of artificial intelligence for materials and chemical discovery; the ability to control coherence in light and matter; the advances in our understanding of quantum systems; and the ability to characterize chemical reactions and pathways far from equilibrium under extreme conditions across multiple length and time scales. These renowned capabilities for the integrated synthesis, characterization, and computational design of new materials and chemical processes have already been brought to bear to accelerate the pace of innovation of net-zero technologies. For example, new battery materials and chemistries, new durable materials for artificial photosynthesis applications, new membranes for hydrogen storage, new recyclable polymers, and new materials exhibiting novel mechanisms for selective capture of CO_2 from flue gas point sources have all been identified, characterized, and understood using DOE's synchrotron light sources, nanoscale research centers, nascent materials databases coupled to machine learning, and state-of-the-art software optimized for DOE's high-performance computing facilities. Despite this progress, significant gaps remain in our **understanding at the electronic and molecular scale, and connecting this understanding to functionality that emerges at larger-length scales.** Investments in addressing these gaps in basic use-inspired science will underpin the development of net-zero technologies. **The science of synthesis, of durability, and of scaling** are all at nascent stages, limiting the efficacy of existing materials and chemical processes for net-zero technologies. For example, research to understand energy transduction at the limits of thermodynamic efficiencies and the kinetics required for direct air CO_2 capture under ultra-dilute conditions are necessary to meet the Biden-Harris goals. To mature and de-risk net-zero technologies at scales sufficient to attract commercial deployment,[8] we must accelerate DOE basic science efforts and strengthen their connection to the development of these technologies in coordination with applied offices within DOE. Capitalizing on these advances to develop better materials, chemistries, and manufacturing processes will require new approaches to teaming among the nation's basic and applied scientists, drawing on cross-Lab expertise and facilities, and an all-of-DOE research network only possible at National Laboratories.

In addition, there is an opportunity to integrate energy systems to optimize their impact. For example, integrating multiple energy sources (such as renewables, nuclear, and low-emissions fossil) and energy forms (e.g., electricity, heat, steam, chemicals) in a hybrid configuration may be beneficial. Fundamental advances are needed to realize **super-efficient multi-input, multi-output (MIMO) net-zero hybrid systems.**[9] New materials, processes, and control methods, such MIMO systems, would utilize a portfolio of energy sources to provide multiple benefits, including flexible output streams, to maximize utilization and profit

8 Davis, S.J., et al. "Net-zero Emissions Energy Systems." *Science* 360 (6396), June 29, 2018: eaas9793. doi: 10.1126/science.aas9793.

9 Arent, et al. "Multi-input, Multi-output Hybrid Energy Systems." *Joule* (2020). https://doi.org/10.1016/j.joule.2020.11.004, accessed January 14, 2021.

across various energy sectors to provide services such as electricity, high-value heat, and chemicals. Combining these capabilities and "systems of systems" design and control innovations would enable **Direct Air Capture**, a promising avenue to remove CO_2 from the atmosphere, to advance, leveraging much-needed research to develop more efficient materials and processes.[10] Utilization of captured CO_2, via not-yet–invented, cost-effective conversion methods is crucial to successfully realize net-zero emissions, circular economy materials pathways, and rejuvenation.

III. Advance Integrated, Scale-Aware Human-Earth Systems Modeling and Observations for Science-Based Decision-Making

The interdependencies in complex, coupled human-Earth systems require science-based analyses of the impacts and risks associated with climate and other environmental changes, as well as the potential efficacy of response strategies. The DOE National Laboratories' sophisticated multisectoral human-Earth systems modeling capabilities are a national set of assets that, if expanded, can support the Biden Administration by providing objective analyses of policies, technologies, and investments aimed at meeting its climate, energy, and environmental equity goals.

Investment and planning decisions for energy systems, critical infrastructure, environmental justice and quality, human health, climate adaptation and mitigation, and other issues often require scientific information about how energy, water, food, infrastructure, land, biological, economic, and climate systems interact across a range of spatial and temporal scales. Some of these complex multiscale interactions are considered by the DOE National Laboratories' integrated human-Earth system models, which represent a broad class of capabilities for understanding, predicting, and mitigating undesirable future changes across a range of climate, energy, and socioeconomic sectors. These models, and associated diverse observations, can be expanded to explore many issues and can be combined with other tools to inform an even broader range of decisions from local to global scales. Past and current applications include evaluation of climate adaptation and mitigation strategies,[11] resiliency assessments,[12] land use and land cover change analysis,[13] impacts on food supply,[14] disease vectors and human health, and technology assessments.[15]

While integrated human-Earth system models provide valuable insights, fundamental challenges remain in the ***science of integrated human-Earth systems; modeling, observational and data science of human-Earth systems across relevant scales;*** and the ***science of multisectoral decision-making.***

The science of integrated human-Earth systems aims to understand how natural and human systems, including the built environment, function and interact. DOE has made enduring investments in research into Earth and human system processes, dynamics, and interactions through its Biological and Environmental Research (BER) program, including two User Facilities aimed at understanding aerosol and cloud processes (the Atmospheric Radiation Measurement User Facility) and biogeochemical processes (the Environmental Molecular Science Laboratory). However, significant knowledge gaps remain, including the likelihood of abrupt and extreme climate transitions; the complete range of often-coupled natural and societal impacts; and the efficacy of adaptation and mitigation measures as the rate of environmental change accelerates, including in natural, managed, and urban systems. Addressing these knowledge gaps requires joint **development of next-generation conceptual and observational systems to underpin the development, calibration, and evaluation of scale-aware human-Earth models.**

Knowledge derived from human-Earth systems research has been incorporated into sophisticated Earth system models, such as the Energy Exascale Earth System Model

10 https://www.nap.edu/catalog/25259/negative-emissions-technologies-and-reliable-sequestration-a-research-agenda, accessed January 14, 2021.

11 Wang T., Z. Jiang, B. Zhao, Y. Gu, K.-N. Liou, N. Kalandiyur, D. Zhang, and Y. Zhu, "Health Co-benefits of Achieving Sustainable Net-Zero Greenhouse Gas Emissions in California." *Nature Sustainability* (2020). [DOI 10.1038/s41893-020-0520-y].

12 U.S. Department of Energy Office of Energy Policy and Systems Analysis, "Climate Change on the U.S. Energy Sector: Regional Vulnerabilities and Resilience Solutions," Oct 2015.

13 Chen, M., C.R. Vernon, N.T. Graham, et al. "Global Land Use for 2015–2100 at 0.05° Resolution under Diverse Socioeconomic and Climate Scenarios." *Sci Data* 7, 320 (2020). https://doi.org/10.1038/s41597-020-00669-x, accessed January 14, 2021.

14 Waldhoff, S.T., I.S. Wing, J. Edmonds, G. Leng, and X. Zhang. "Future Climate Impacts on Global Agricultural Yields over the 21st Century." *Environmental Research Letters* 15, no. 11 (October 21, 2020): 114010. https://iopscience.iop.org/article/10.1088/1748-9326/abadcb, accessed January 14, 2021.

15 Daioglou, V., S.K. Rose, N. Bauer, et al. "Bioenergy Technologies in Long-run Climate Change Mitigation: Results from the EMF-33 Study." *Climatic Change* 163, 1603–1620 (2020). https://doi.org/10.1007/s10584-020-02799-y, accessed January 14, 2021.

(E3SM),[16] and integrated human-Earth system models, such as the Global Change Analysis Model (GCAM).[17] Each of these capabilities has steadily increased in its complexity and resolution, and GCAM is now included within E3SM to provide a comprehensive capability for predicting the future evolution of the coupled human-Earth system under different scenarios. Improvements in the utility of these models can be achieved through multi-scale **representations** of climate-related human health impacts, population dynamics, and urbanization trends; energy, water, and agricultural strategies; environmental equity factors; environmental impacts; and emerging zero- and negative-emission technologies. As the models become more complex, additional **improvements in their speed, uncertainty quantification, and ability to rapidly assimilate diverse observations will be required, as well as their ability to perform large ensemble simulations.**

Also required are advancements in human-Earth systems data science to make data readily interpretable to scientists and policy makers and more rapidly incorporated into next-generation models. The science of multisectoral decision-making applies integrated human-Earth systems models to analyze and assess climate vulnerabilities, resiliency, and risks associated with various technology, policy, and investment options. Integrated human-Earth system models have predicted the timing, frequency, and severity of extreme events,[18] the impacts and timing of Arctic sea ice decline and permafrost thaw,[19] future water availability[20] and drought,[21] and temperature changes on a global and regional basis.[22] Information provided by these predictions and analyses could enable communities to develop strategies to enhance their resilience or inform community relocation programs, infrastructure design, and adaptation strategies.

Models have also been used to assess the vulnerability and resilience of the nation's energy system under changing regional climate conditions, but they could be extended to evaluate adaptation and mitigation options, costs, and benefits, including human health and social and environmental equity implications. **Increasing the fidelity and utility of human-Earth model projections and their application to decision-making** would ultimately deliver a science-based approach to developing a clear vision for resilient communities and ecosystems.

To inform the development of sustainable solutions to the nation's energy and environmental challenges, there is a significant opportunity to advance observational, data, and modeling of human-Earth system capabilities through partnerships across many DOE offices. Examples include DOE-OE (whose remit is to ensure a resilient and reliable grid), DOE-CESER (which includes emergency response), and EERE-AMO (which has recently made a large investment in water-energy systems through the NAWI Hub). ASCR-supported expertise will be required to propel advances in artificial intelligence, machine learning, edge computing, and the 5G capabilities needed to identify non-obvious predictors and precursors of human and Earth system phenomena. This expertise also will enable large ensemble simulations for scenario analysis and uncertainty assessments, and quickly assimilate diverse datasets to enable rapid evaluation of strategies, system response to extreme events, and near-real-time decision-making.

The DOE National Laboratories' science-based multisectoral human-Earth systems modeling capabilities can provide decision-makers with a powerful capability to evaluate and prioritize investments and programs that address multiple policy-related goals and outcomes simultaneously. Being able to objectively weigh the ramifications of decisions made in the context of complex, coupled human-Earth systems will position the U.S. to develop effective climate mitigation and resilience strategies that also meet our nation's energy and environmental equity objectives.

16 https://e3sm.org/, accessed January 14, 2021.

17 http://www.globalchange.umd.edu/gcam/, accessed January 14, 2021.

18 Balaguru, K., G.R. Foltz, and L.R. Leung. "Increasing Magnitude of Hurricane Rapid Intensification in the Central and Eastern Tropical Atlantic." *Geophysical Research Letters,* 45, 4238 – 4247 (2018). https://doi.org/10.1029/2018GL077597, accessed January 14, 2021.

19 Zou, Y., Y. Wang, Z. Xie, H. Wang, and P.J. Rasch, "Atmospheric Teleconnection Processes Linking Winter Air Stagnation and Haze Extremes in China with Regional Arctic Sea Ice Decline." *Atmospheric Chemistry and Physics,* 20, 4999–5017 (2020). [DOI: 10.5194/acp-20-4999-2020]

20 Graham, N.T., M.I. Hejazi, S. H. Kim, et al. "Future Changes in the Trading of Virtual Water." *Nat Commun* 11, 3632 (2020). https://doi.org/10.1038/s41467-020-17400-4

21 Yoon, J.-H., S.-Y. Simon Wang, R.R. Gillies, B. Kravitz, L. Hipps, and P.J. Rasch. "Increasing Water Cycle Extremes in California and Relation to ENSO Cycle under Global Warming." *Nature Communications,* Oct. 21 (2015) [DOI: 10.1038/ncomms9657]

22 Snyder, A., R. Link, K. Dorheim, B. Kravitz, B. Bond-Lamberty, and C. Hartin. "Joint Emulation of Earth System Model Temperature-Precipitation Realizations with Internal Variability and Space-time and Cross-Variable Correlation: Fldgen v2.0 Software Description." *PLOS ONE* 14(10): e0223542 (2019). [DOI: 10.1371/journal.pone.0223542]

IV. Develop an Integrated Land-based Negative Emissions Bioenergy Economy

The Earth's terrestrial ecosystems absorb roughly one-third of all anthropogenic CO_2 emissions from the atmosphere each year, providing a valuable carbon sink that is on par with the most aggressive climate mitigation measures that are being pursued. Plants naturally capture, store, and convert CO_2 through photosynthesis and build above- and below-ground natural carbon pools. Soils hold ~3 times more carbon than does the atmosphere.[23] Current greenhouse reduction strategies assume that terrestrial ecosystems will continue to serve as a significant carbon sink. However, a predictive understanding of the propensity of terrestrial ecosystems to serve this role under future climates is limited. In response, BER initiated the Next Generation Ecosystem Experiment (NGEE) projects to develop a predictive understanding of terrestrial carbon sinks focused on the most vulnerable natural ecosystems.[24] Other DOE programs, such as the DOE Bioenergy Research Centers, the BES Energy Frontier Research Centers, and multiple programs in DOE-BETO, are developing technologies capable of capturing and converting CO_2 into biofuels and bioproducts. All told, these efforts present a significant opportunity to advance transformative, land- and manufacturing-based negative emissions technologies (NETs), also referred to as carbon dioxide removal (CDR) strategies, which are required to meet targets identified by IPCC and the Biden-Harris Administration.

Effective land-based NET strategies must consider fundamental abiotic reactions and microbe-soil-plant interactions and their manifestation at larger scales within heterogeneous ecosystems and their behaviors under future climates. Recent reports have identified anthropogenically enhanced soil mineralization (for example, adding finely ground basalt to crop land) as one of the most promising early-stage research targets, potentially leading to 2–4 Gt of CO_2 removal per year globally.[13] Accrual of soil carbon could represent 25% of the total potential of natural climate solutions, 60% of which could be realized by rebuilding depleted subsurface stocks, and comprises 47% of the mitigation potential for agriculture and grasslands globally.[25] Soil carbon sinks offer a much larger (perhaps >10x) offset potential than forests, which account for 95% of the carbon offsets today. While not yet explored, there is a significant opportunity to advance and integrate genomic (including synthetic biology) with ecosystem approaches to accelerate terrestrial system CDR in both natural ecosystems and working lands.

Sustainable management of plants and microbes used to regenerate natural carbon sinks can contribute to negative emissions when combined with energy generation, sequestration, and carbon utilization in bio-advantaged fuels, durable products, and biopower. Incorporating greater use of CO_2 into the bioeconomy is a clear opportunity to remove carbon from the atmosphere while creating new jobs and strengthening the U.S. economy. Bioenergy Carbon Capture and Storage, or BECCS, is a CDR strategy that relies on: (1) conversion of biomass, derived largely from rapidly growing trees or grasses, into heat, electricity, liquid or gas fuels, or bioproducts; (2) the capture of carbon emissions associated with bioenergy production; and (3) the storage of CO_2 in soils, geological formations, or in long-lasting products.[13]

Retrofitting existing coal-fired power plants to burn biomass — piloted in the UK — represents a potentially large opportunity for biopower with BECCS deployment. Moreover, BECCS is currently the most economical and technologically advanced option, and the agriculture and forestry sector workforce could be readily deployed to implement these techniques.

Approximately 13% of the U.S. land surface is presently categorized as degraded (marginal) land.[26] These lands, often low in nutrients and prone to drought, represent an opportunity to expand the U.S. Bioeconomy. **Soil enhancement strategies** can lead to benefits beyond carbon reduction, including improved soil fertility important for food and bioenergy crops, and beneficial use of mining and other wastes. **Plants that can withstand water limitations, efficiently acquire nutrients from low-fertility soils, and are facilitated by microbial fixation of nitrogen** would pave the way for sustainable cropping systems to underpin the U.S. bioenergy economy. A more diversified landscape that intentionally utilizes marginal agricultural land to produce bioenergy side-by-side with current agricultural commodities also has the potential to cost-effectively remove excess nutrients from water, mitigating Gulf of Mexico hypoxia and algal blooms elsewhere, as

23 Hepburn, C., et al. "The Technological and Economic Prospects for CO2 Utilization and Removal." *Nature,* 575, 87 (2019). https://doi.org/10.1038/s41586-019-1681-6, accessed January 14, 2021.

24 Next-Generation Ecosystem Experiments-Arctic (https://tes.science.energy.gov/research/ngeearctic.shtml) and Next Generation Ecosystem Experiments-Tropics (https://tes.science.energy.gov/research/ngeetropics.shtml), both accessed January 14, 2021

25 Bossio, D.A., *et al.* "The Role of Soil Carbon in Natural Climate Solutions." *Nature Sustainability* 3, 391-398 (2020).

26 https://www.nrel.gov/docs/fy10osti/46209.pdf, accessed January.

well as reduce over-use of important water resources. Rural communities could reap opportunities to become environmental entrepreneurs, while at the same time produce biomass for energy and bioproducts.

Finally, monitoring methods are needed to track land-based carbon stabilization over a range of space and time scales, and at accuracies that allow for carbon quantification and credit accounting. The DOE AmeriFlux observational network, which consists of towers that measure carbon and other fluxes, is distributed across the nation but currently not at a density needed for carbon tracking. There is a significant opportunity to take advantage of **rapidly developing sensors, drones, satellites, 5G, and AI techniques** to advance a robust CO_2 and methane-sensing strategy for the nation.

Development of an integrated, land-based, negative emissions bioenergy economy requires an investment in RD&D **to address fundamental questions and overcome technological barriers and scale-up challenges.** The fundamental questions and ability to acquire knowledge of **microbe-soil-plant interactions across needed scales** are best addressed through tightly integrated laboratory experiments from molecular to mesoscales, multi-scale simulations, and in-situ field studies performed in natural and managed ecosystems over scales and conditions that are representative of the complexity of deployment scenarios. Advancements in artificial intelligence and machine learning have the potential to accelerate the development of biological solutions for carbon capture and conversion into fuels and products. DOE is in a unique position to lead these efforts by leveraging expertise in both large-scale ecological manipulation and ecosystem studies, as well as existing User Facilities.

LABORATORIES AND DIRECTORS (AS OF JANUARY 2021)

DOE LABORATORY CONTRACTOR	**DIRECTOR**
Ames Laboratory Iowa State University of Science & Technology	**Adam Schwartz**
Argonne National Laboratory (ANL) UChicago Argonne, LLC	**Paul Kearns**
Brookhaven National Laboratory (BNL) Brookhaven Science Associates, LLC	**Doon Gibbs**
Lawrence Berkeley National Laboratory (LBNL) University of California	**Michael Witherell**
Fermi National Accelerator Laboratory (FNAL) Fermi Research Alliance, LLC	**Nigel Lockyer**
Idaho National Laboratory (INL) Battelle Energy Alliance, LLC	**John Wagner**
Los Alamos National Laboratory (LANL) Triad National Security, LLC	**Thom Mason**
Lawrence Livermore National Laboratory (LLNL) Lawrence Livermore National Security, LLC	**William (Bill) Goldstein**
National Energy Technology Laboratory (NETL) Government-owned, government-operated	**Brian Anderson**
National Renewable Energy Laboratory (NREL) Alliance for Sustainable Energy, LLC	**Martin Keller**
Oak Ridge National Laboratory (ORNL) UT-Battelle, LLC	**Thomas Zacharia**
Pacific Northwest National Laboratory (PNNL) Battelle Memorial Institute	**Steven Ashby**
Princeton Plasma Physics Laboratory (PPPL) Princeton University	**Steve Cowley**
Sandia National Laboratories (SNL) National Technology and Engineering Solutions of Sandia, LLC	**James Peery**
Savannah River National Laboratory (SRNL) Savannah River Nuclear Solutions, LLC	**Vahid Majidi**
SLAC National Accelerator Laboratory Stanford University	**Chi-Chang Kao**
Thomas Jefferson National Accelerator Facility (TJNAF) Jefferson Science Associates, LLC	**Stuart Henderson**
NLDC Secretariat	**Julie Wulf-Knoerzer**

CONTACT
Doon Gibbs
Chair
National Laboratory Directors' Council
Email: gibbs@bnl.gov