Recommendations for Strengthening American Leadership in Industries of the Future

A Report to the President of the United States of America

The President's Council of Advisors on
Science and Technology

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About this Document

At its meeting in November, 2019, PCAST agreed to undertake a process to develop a set of bold recommendations to help ensure continued American leadership in Industries of the Future (which comprise artificial intelligence, quantum information science, advanced manufacturing, advanced communications networks, and biotechnology). This report is the culmination of that process.

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California Institute of Technology

Subject Matter Experts

Grace Diana
OSTP

Matt Wilson
OSTP

Cindy Hasselbring
OSTP

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Abbreviations and Acronyms

ACD	Advisory Committee to the Director
AI	artificial intelligence
AIBLE	Artificial Intelligence for BiomedicaL Excellence
AITO	Artificial Intelligence and Technology Office
ARPANET	Advanced Research Projects Agency Network
ASCR	Advanced Scientific Computing Research
BIOME	Biotechnology Institute of Manufacturing Excellence
CORD-19	COVID-19 Open Research Dataset
CRENEL	Commission to Review the Effectiveness of the National Energy Laboratories
DARPA	Defense Advanced Research Projects Agency
DoD	Department of Defense
DOE	Department of Energy
DOT	Department of Transportation
ESIX	Economic and Security Implications of Quantum Science
FAA	Federal Aviation Administration
FAB	Foundries for American Biotechnology
FDA	Food and Drug Administration
FotF	Factories of the Future
FY	fiscal year
GPU	graphics processing unit
GSA	General Services Administration
HHS	Department of Health and Human Services
HPC	high performance computing
IotF	Industries of the Future
IP	intellectual property
IT	information technology
ITEST	Innovative Technology Experiences for Students and Teachers
JAIC	Joint AI Center
JSEP	Joint Services Electronics Program
MGI	Materials Genome Initiative
ML	machine learning
NBI	National Biodesign Institute
NBiotA	National Biotechnology Accelerator
NIH	National Institutes of Health
NIST	National Institute of Standards and Technology
NITRD	Networking and Information Technology Research and Development Program
NSB	National Science Board
NSCI	National Strategic Computing Initiative
NSF	National Science Foundation
NSTC	National Science and Technology Council
NVBL	National Virtual Biotechnology Laboratory
OECD	Organisation for Economic Co-operation and Development
OSTP	Office of Science and Technology Policy
PCAST	President's Council of Advisors on Science and Technology
QCLI	Quantum Leap Challenge Institutes
QED-C	Quantum Economic Development Consortium
QIS	quantum information science

QISE-Net Quantum Information Science and Engineering Network

QLCI Quantum Leap Challenge Institutes

QRC quantum research collaboration

R&D research and development

SCQIS Subcommittee on Quantum Information Science

SRC Semiconductor Research Corporation

STEM science, technology, engineering, and mathematics

TOPS tera operations per second

U.S. United States

USA United States of America

USDA U.S. Department of Agriculture

Executive Summary

The President's Council of Advisors on Science and Technology (PCAST) is recommending a set of bold actions to help ensure continued American leadership in Industries of the Future (IotF, comprising artificial intelligence (AI), quantum information science (QIS), advanced manufacturing, advanced communications, and biotechnology). The three pillars underpinning these actions are (a) enhancing multi-sector engagement in research and innovation; (b) creating a new institute structure that integrates one or more of the IotF areas and spans discovery research to product development; and (c) creating new modalities for ensuring the availability of a qualified, diverse IotF workforce.

With regard to the first pillar, Federal agencies need to take full advantage of their administrative authorities to partner with industry and academia in new and innovative ways, particularly to ensure the effective transition and translation of early-stage research outcomes into applications at scale. In the area of AI, this includes establishing a joint AI Fellow-in-Residence program, AI Research Institutes in all 50 States, National AI Testbeds, partnerships for curating and sharing large datasets, and joint international programs for attracting and retaining the best global talent, and research and development (R&D) and training for trustworthy AI.

In the area of QIS, industry participation is critically important in building world-class quantum infrastructure at scale, particularly quantum computing systems, and a quantum internet and intranet. Federal investments are needed to establish national quantum computing user facilities, educate a quantum workforce, create pre-competitive quantum research collaborations, establish quantum foundational discovery institutes, and to attract and retain the best global talent.

The second pillar of this report homes in on a new model for leveraging the strength of America's National Laboratories to enhance and accelerate substantial front-to-back progress in IotF. The cornerstone recommendation involves establishing a new type of world-class, multi-sector R&D institute that catalyzes innovation at all stages of R&D—from discovery research to development, deployment, and commercialization of new technologies. These highly prestigious "IotF Institutes" would support portfolios of collaborative projects at the intersection of two or more IotF pillars, and be structured to minimize burdensome administrative overhead so as to maximize rapid progress. They would utilize innovative intellectual property terms that incentivize participation by industry, academia, and non-profits as a means for driving commercialization of IotF technologies at scale. Importantly, these institutes would be located to maximize multi-sector collaboration and the ability to function as regional hubs for technological, economic, and skill development via Opportunity Zones, HUBZones, and other relevant programs.

We identify two areas as candidates for initial flagship institutes. The first would focus on the integration of AI and advanced manufacturing, while the second would combine AI and biotechnology to enhance biosecurity, biosafety, and biosphere sustainability.

Achieving success with the first two pillars of this report rests upon the Nation's ability to strengthen, grow, and diversify its science, technology, engineering, and mathematics (STEM) workforce at all levels—from skilled technical workers to researchers with advanced degrees. First and foremost, America must build the Workforce of the Future by creating STEM training and education opportunities for individuals from all backgrounds, STEM and non-STEM, including underrepresented and underserved populations. Employers, academic institutions, professional societies, and other partners should develop programs to provide non-STEM workers with professional competencies that will grant them a role in the STEM Workforce of the Future. Public- and private-sector employers should be recruited to pledge and realize support for hiring newly skilled STEM workers, especially those from non-traditional backgrounds, into STEM positions. And the National Science Foundation should establish a grant program to create and pilot multi-sector, Workforce of the Future STEM Retraining Boards that connect individuals to new or existing opportunities for continuing education, training, certification, and reskilling in STEM fields.

In addition, curricular innovations, and universal skills-based licenses and certifications are required for America to continue leading the world in IotF. Specifically, Federal funds, matched by support from the private sector and universities, are needed to create industry-recognized curricula and work-based learning and training programs in QIS, AI, and advanced manufacturing. Structured as public-private partnerships, these efforts should yield universal skills-based licenses and certifications targeting IotF. Employers should commit to using skills-based certifications as the basis for training/education and job descriptions, using informed recommendations from industry and professional societies. These activities are ever more urgent today for getting individuals back to work in the face of COVID-19, and for empowering individuals to work and thrive in these emerging IotF.

The principles and recommendations contained in this report are interconnected and mutually reinforcing, designed to bridge these pillars and harness key opportunities for the Nation. PCAST believes that the cross-sector actions recommended herein will lay a strong foundation for sustaining U.S. discovery, innovation, and prosperity well into the future.

Introduction

For many decades, the United States has been a global leader in science and technology (S&T). This exceptional foundation of research and development (R&D)—which underpins our Nation's security, health, economic strength, and innovation enterprise—traces its origin to the period immediately following World War II, empowered in large part by Vannevar Bush's visionary treatise, *Science: The Endless Frontier*.[1] This and other actions created the First Bold Era of Science and Technology in America, built on a four-sector ecosystem spanning the Federal Government, the private sector, universities, and non-profit organizations. Collectively, this ecosystem today expends some $600 billion each year on R&D. Maintaining leadership in S&T is of critical importance to the future of America as it enters a Second Bold Era of Science and Technology. This era is marked by great challenge as other nations advance rapidly, yet it also is marked by great promise.

Consequently, new ways of thinking and working are required to maintain America's preeminence, including new collaborative initiatives that leverage our substantial assets; multi-sector partnerships that bring the best ideas, capabilities, and people to the table; and strategies for greatly accelerating progress and removing barriers to innovation. Additionally, America must leverage the full potential of its human resources by overcoming historical barriers that have limited inclusion of individuals in STEM. Broadening access to those who are in underrepresented and underserved communities—including those who have been displaced by COVID-19 pandemic-related economic disruption—can unleash new potential and create pathways to economic prosperity for all, while helping to meet critical workforce needs.

Among the greatest challenges America faces are questions of not only how to maintain, but also enhance its global leadership in Industries of the Future (IotF). IotF encompasses artificial intelligence (AI), quantum information science (QIS), advanced manufacturing, advanced communications (5G and beyond), and biotechnology. Nothing has put a finer point on this issue than the COVID-19 pandemic, where the benefits of IotF are ubiquitous and compelling. They range from technologies supporting remote learning and enhanced capabilities in medicine and telemedicine, to the rapid production of medical counter-measures to the synthesis of more than 130,000 publications that have greatly accelerated scientific progress on both the virus and its associated disease.[2] They also include modeling and prediction of disease spread, assessing the potential for disease severity based upon underlying comorbidities and other factors, and rapidly comparing this coronavirus with thousands of other viruses in databases worldwide.

It is with this compelling need in mind, and also the opportunity and obligation now before us, that the President's Council of Advisors on Science and Technology (PCAST) recommends a set of bold actions to help ensure continued American leadership in IotF. The three pillars underpinning these actions are (a) enhancing multi-sector engagement in research and innovation; (b) creating a new institute structure that integrates one or more of the IotF areas and spans discovery research to product development; and (c) creating new modalities for ensuring the availability of a qualified, diverse IotF

[1] Bush, Vannevar. 1945. *Science: The Endless Frontier: a Report to the President on a Program for Postwar Scientific Research*. July 1945. National Science Foundation. See also the new 75th Anniversary Edition, released by the National Science Foundation (NSF) in celebration of NSF's 70th Anniversary: https://www.nsf.gov/about/history/EndlessFrontier_w.pdf

[2] The COVID-19 Open Research Dataset, known as CORD-19, included over 130,000 scientific articles about the SARS-CoV-2 virus as well as related viruses in the broader coronavirus group as of June 28, 2020. More information can be found at https://www.semanticscholar.org/cord19

workforce. The principles and recommendations contained in this report are interconnected and mutually reinforcing, designed to bridge these pillars and harness key opportunities for the Nation. Education, workforce, and diversity and inclusion recommendations are offered throughout this report, with additional specific recommendations provided in the final section. PCAST believes that the cross-sector actions recommended herein will lay a strong foundation for sustaining U.S. discovery, innovation, and prosperity well into the future.

1. Enhancing Multi-Sector Engagement in IotF Research and Innovation

A key priority for the Nation is advancing the IotF—namely, AI, QIS, advanced manufacturing, advanced communications (5G and beyond), and biotechnology—to keep the United States at the leading edge of scientific discovery. The COVID-19 pandemic has revealed the essential role of IotF in empowering the Nation to respond to the ongoing global health crisis.

In the following section, this report explores strategies for enhancing cross-sector and international cooperation for accelerating progress in IotF, with a particular emphasis on AI and QIS. PCAST proposes new systems of collaboration between government, industry, academia, and non-profit S&T organizations. In addition to proposing actions that will allow the United States to maintain its leadership in IotF, PCAST sees enormous opportunity to accelerate scientific discovery by combining the power of AI, QIS, and high-performance computing (HPC). PCAST also sees a critical need to prepare the American workforce at all levels for the growth of AI and QIS in the coming years.

Artificial Intelligence

Over the last decade, AI—especially machine learning (ML)—has emerged as one the most important technologies of our era. AI touches nearly every aspect of modern society, from our daily lives to business operations to how research is performed. Advancing rapidly as a technological force, AI is affecting all industries and economies. Powered by exponential growth in computing infrastructure and ever-increasing availability of data, technological breakthroughs in AI are enabling intelligent systems to take on increasingly sophisticated tasks and augment human capabilities in new and profound ways.

In recent months, during the COVID-19 crisis, AI has demonstrated critical capabilities as well as important potential for the future. For example, AI has been essential in acquiring knowledge and performing in-depth searches of the numerous scientific articles related to the virus, disease, and pandemic. Government, industry, and academia worked together to release over 130,000 scientific articles and issued a call to action[3] to the AI community to develop AI tools and techniques that can analyze the corpus.[4] AI also has been used in fundamentally new ways, such as in the creative design and efficient screening of molecules for their potential ability to bind to and interrupt functional target sites of the SARS-CoV-2 coronavirus.

The United States is at a critical juncture in advancing AI to achieve further breakthroughs such as these, as well as to maintain leadership in AI. This is essential for driving advances needed for COVID-19, enhancing preparedness for future pandemics, as well as bolstering the Nation's success in IotF. But American leadership it is not assured. Globalized access to information and accelerated technology adoption are collapsing the timescale for innovation—AI in particular is advancing at a pace not seen in any technological field in the last century. The advances in AI that are powering today's rapid progress are originating around the globe, and the United States cannot risk falling behind.

The United States will need to move swiftly to increase investment and restructure its R&D partnerships across industry, academia, and government, and with other nations. The United States also will need to move quickly to address AI skills shortages in the workforce.

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[3] https://www.whitehouse.gov/briefings-statements/call-action-tech-community-new-machine-readable-covid-19-dataset/

[4] https://www.kaggle.com/allen-institute-for-ai/CORD-19-research-challenge; https://www.semanticscholar.org/cord19

Industry, academia, and government should dramatically expand their AI R&D to power the Nation to continue to lead in AI S&T—to provide a robust foundation for U.S. industry to compete at a global scale, and to ensure national prosperity and security. This report offers critical recommendations to accelerate basic science and translational R&D, as well as to greatly expand investment in infrastructure, partnerships, work-based learning opportunities, training, and education. By accelerating the pace of innovation in basic research, creating programs and infrastructure that drive the translation of innovation and capture feedback from its applications, and ensuring the Nation has the required skills and talent, the United States will be strongly positioned to leverage a new robust foundation for accelerating scientific discovery and leading globally in the future AI industry.

Background on Federal AI Actions

The recommendations of this report are intended to augment or strengthen Federal actions on AI. Recent activity includes a White House Summit on Artificial Intelligence,[5] establishment of the Select Committee on Artificial Intelligence[6] within the National Science and Technology Council (NSTC), the launch of the American AI Initiative,[7] and updating of the National AI R&D Strategic Plan.[8] In addition, The White House issued a request for information asking for comments on the need for additional access to Federal data and models, established the Federal Data Strategy,[9] and took steps to leverage computing resources for AI applications.

In parallel, Federal regulatory agencies have been adopting new guidance and frameworks for AI. The Department of Transportation (DOT) issued updated guidance for automated vehicle technologies; the Federal Aviation Administration (FAA) enabled previously prohibited autonomous aircraft operations; and the Food and Drug Administration (FDA) proposed a regulatory framework for AI-based medical software. In parallel, proposed United States AI Regulatory Principles[10] were published and the National Institute of Standards and Technology (NIST) issued a strategy for Federal engagement in the development of AI technical standards.[11]

Internationally, the United States led efforts at the Organisation for Economic Co-operation and Development (OECD) to develop the first international consensus agreements[12] on fundamental principles for the stewardship of trustworthy AI. Additionally, the United States joined the G7 nations in launching the Global Partnership on Artificial Intelligence.

Workforce development actions have included direction to all Federal agencies to prioritize AI-related apprenticeship and job training programs. New programs such as the National Science Foundation's (NSF) National AI Research Institutes program[13] aim to contribute to the training of PhD-level AI researchers.

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5 https://www.whitehouse.gov/wp-content/uploads/2018/05/Summary-Report-of-White-House-AI-Summit.pdf
6 https://www.whitehouse.gov/wp-content/uploads/2018/05/Summary-Report-of-White-House-AI-Summit.pdf#page=13
7 https://www.whitehouse.gov/articles/accelerating-americas-leadership-in-artificial-intelligence/
8 https://www.whitehouse.gov/wp-content/uploads/2019/06/National-AI-Research-and-Development-Strategic-Plan-2019-Update-June-2019.pdf
9 https://strategy.data.gov/
10 https://www.whitehouse.gov/wp-content/uploads/2020/01/Draft-OMB-Memo-on-Regulation-of-AI-1-7-19.pdf
11 https://www.nist.gov/system/files/documents/2019/08/10/ai_standards_fedengagement_plan_9aug2019.pdf
12 http://www.oecd.org/going-digital/ai/principles/
13 https://www.nsf.gov/news/news_summ.jsp?cntn_id=299329&org=NSF&from=news

AI R&D Investment Trends in the United States

AI has the potential not only to transform S&T, speeding up the pace of scientific discovery and technical innovation, but also to improve essential activities, such as developing solutions to COVID-19. It has the potential to contribute to the discovery of new therapies and accelerate their translation to novel treatments in healthcare, boost the accuracy of medical diagnoses, and broadly improve the delivery of healthcare and lower costs, all through effective data-driven solutions. AI can create resilient cyber-physical systems and transform national defense and security. However, fully seizing the opportunities presented by AI requires a robust collaboration among industry, academia, and government, facilitated by significant and sustained investments to address research and workforce development challenges.

In recent years, building upon decades of prior investments in long-term basic research by the Federal Government, U.S. industry has made massive investments that have driven U.S. technology leadership. Five of the top industry technology leaders (Amazon, Facebook, Google, IBM, and Microsoft) spent over $65 billion in R&D in 2018, which is roughly half that of the Federal Government.[14] A large and growing portion of this spending involves work in AI. From 2020–2025, it is reasonable to estimate yearly U.S. industry investments in AI R&D will exceed $100 billion.

PCAST believes expanded Federal investments are needed to lay the foundation for future transformative discoveries in AI and for continued innovation in and investment by the private sector. The Fiscal Year (FY) 2021 President's Budget proposes doubling non-defense AI R&D spending by FY 2022 compared to FY 2020. If enacted, annual spending for AI R&D would total more than $2 billion by FY 2022. The Department of Defense (DoD) allocated $4 billion toward AI/ML R&D activities in FY 2020. The cornerstone of the Pentagon's AI program, the Joint AI Center, or JAIC, received $209 million of that funding.[15]

PCAST believes the United States should continue to balance AI R&D across near-term and long-term goals by growing Federal investment in both fundamental research and translational efforts across academia, government, and industry. Increased coordination and collaboration among academic institutions, National Laboratories, and industry will be a cornerstone to drive progress, as described further in Section 2. Economies of scale can be achieved by sharing resources, materials, data, and infrastructure. More broadly, identifying and replacing duplication with synergistic, streamlined activities could enhance the combined capability and result in significant cost savings that could then be reinvested in the research enterprise.

An important opportunity for America during the next 5 years involves building focused partnerships with industry to advance the Nation's AI R&D infrastructure, creating an open technical foundation for AI, and improving AI skills of the U.S. workforce. Collectively, they represent investments at the multi-billion-dollar level. Industry contributions could take the form of free compute infrastructure grants for academia, corporate-backed open source software, open publications, sponsored university programs, and education in AI. Such investments would constitute a significant contribution to a multi-sector partnership for accelerating the Nation's pace of innovation in AI—an investment the Federal Government has an opportunity to scale and amplify through a set of complementary actions.

[14] National Science Board | Science & Engineering Indicators | NSB-2020-5 (https://ncses.nsf.gov/pubs/nsb20205)

[15] Bloomberg Government https://about.bgov.com/news/finding-artificial-intelligence-money-fiscal-2020-budget/

Recommendations

As noted previously, the United States should continue to increase investment in AI and leverage new partnerships across industry, academia, and government[16] to achieve and sustain global leadership. Specifically, bold action should be taken jointly, where industry, academia, and government are stakeholders across all these areas (principal responsibility is indicated as I = industry, A = academia, and G = government). PCAST's recommendations address only non-defense AI R&D. For an assessment of defense and national security AI R&D needs and opportunities, refer to the important November 2019 Interim Report of the National Security Commission on Artificial Intelligence[17] and to the recommendations this commission will make in their final report.

Recommendation 1.1: ***Grow Federal investment in AI R&D by a factor of 10 over 10 years. (G)***

New and sustained research in AI is required to drive major S&T progress over the next decade. This includes development and deployment of advanced systems that learn and reason broadly so they can partner with and augment human capability to take on increasingly complex and valuable tasks. To achieve that goal, and in addition to the estimated $100 billion of U.S. industry investments in AI from 2020–2025, PCAST recommends growing federally funded non-defense AI R&D by a factor of 10 over the next 10 years.

Table 1. *Proposed Federal Budget Ramp for Non-Defense AI Research*

2020	2022[18]	2024	2026	2028	2030
$1 billion	$2 billion	$4 billion	$6 billion	$8 billion	$10 billion
Consistent with the President's FY 2021 Budget		Recommending sustained investment growth of $1 billion/year in non-defense research funding through 2030			

This action is required to support rapid progress in critical areas of fundamental AI research[19] and to advance AI technology beyond today's capabilities. This should be accomplished, in part, by expanding the programmatic funding of existing offices, directorates, and programs that support AI R&D at NSF, the National Institutes of Health (NIH), NIST, and the Department of Energy (DOE). This investment should allow for programs that support small teams of investigators to work on specific problems, as well as programs that support larger grants and institutional centers. This funding increase would enable the expansion of work on important core problems, such as making AI learn from smaller amounts of data; developing causal-inferencing AI; creating trustworthy AI; developing AI engineering methodologies that allow greater scaling of AI applications; and developing new approaches for AI

[16] https://uidp.org/publication/broadening-university-industry-engagement-symposium-report/
[17] https://www.nscai.gov/about
[18] https://www.whitehouse.gov/wp-content/uploads/2020/02/ap_17_research_fy21.pdf
[19] As consistent with the *National AI R&D Strategic Plan: 2019 Update*. https://www.nitrd.gov/pubs/National-AI-RD-Strategy-2019.pdf

hardware in the post-graphics processing unit era.[20] It also should bolster support for basic research on cross-cutting areas such as AI security and vulnerability; connectivity and communications; data curation and governance; privacy and ethics; and the implementation of associated best practices. Additional recommendations for NSF, NIH, and DOE are provided below.

NSF Opportunities. The FY 2020 President's Budget for AI R&D within NSF is $487 million.[21] Based on the number of highly rated proposals that currently go unfunded but are of equal merit to those which are funded, PCAST anticipates that growing the investment to $1 billion would allow for making at least 1,000 additional awards to individual investigators without any loss of quality. Increasing support for human capital by expanding the pool of NSF-funded investigators will accelerate the pace of discovery and growth of AI solutions across the board. Increased investment levels would further allow the expansion of NSF's flagship National AI Research Institutes. In 2020, six such institutes were selected for investment, each at $20 million over 5 years.

PCAST believes it necessary for every State to have at least one AI institute, which would require a net investment of $1 billion over 5 years. The broad expansion of AI institutes would allow for a foundation of AI expertise and specialization to best match the needs of each State. These institutes should be operated in a networked fashion to create National AI Consortia to enable sharing of best practices and mutual benefit from shared infrastructure, such as data and computation resources.

NIH Opportunities. The FY 2020 President's Budget for AI R&D within NIH is $202 million.[22] Much of the prior AI R&D at NIH has focused on text mining, genomic medicine (development of large genomic databases, dbSNP), image processing, and behavioral research. NIH clearly recognizes the potential of applying ML to biomedical data to enable major societal benefits, ranging from biomedical discoveries and enhancement and individualization of clinical care, to improvements in health delivery and practice at the community level.

However, although NIH generates large amounts of data, several challenges exist in linking them effectively with AI data analysis and discovery tools. Specifically, NIH does not own much of the data generated by its research funding, and the data it does have often and understandably are subject to privacy and other restrictions. Further, the agency does not operate or maintain computer facilities, and most of its data are not in a form suited for ML and inference. The NIH Advisory Committee to the Director (ACD) on AI Working Group recently released a report recognizing these challenges.[23] Its recommendations focus on data generation, curation, accessibility, and dissemination, as well as regulatory, ethical, and privacy standards. NIH is setting up the Artificial Intelligence for BiomedicaL Excellence (AIBLE) program, a new NIH-wide Common Fund initiative that will generate new biomedically-relevant data sets amenable to ML analysis at scale. PCAST believes this program has been thoughtfully conceived, but at the current level of investment will only be able to tackle one problem at a time (one data design center is planned per year). Given the ambitious objectives to scale

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[20] A graphics processing unit (GPU) is a specialized electronic circuit designed for specific workloads, such as calculations related to 3D computer graphics. During the last decade they have been broadly used for deep learning workloads, which are core to recent AI advances.

[21] NITRD Budget Supplement: The Networking & Information Technology Research and Development Program Supplement to the President's FY2020 Budget. September 2019. National Science & Technology Council, Washington, DC. https://www.nitrd.gov/pubs/FY2020-NITRD-Supplement.pdf

[22] NITRD Budget Supplement: The Networking & Information Technology Research and Development Program Supplement to the President's FY2020 Budget. September 2019. National Science & Technology Council, Washington, DC. https://www.nitrd.gov/pubs/FY2020-NITRD-Supplement.pdf

[23] https://acd.od.nih.gov/documents/presentations/12132019AI_Report.pdf

up and amplify this effort by funding multiple data design centers that operate in parallel, funding levels need to be increased by at least an order of magnitude to have impact at scale.

PCAST further believes it essential that NIH strengthen its partnerships with academia, industry, and other Federal agencies (such as DOE, NSF, and NIST) to enable it to meet the defined goals. For instance, in the context of the current COVID-19 pandemic, there is an urgent need for the vast and highly significant amounts of data currently being generated to be made AI-ready from the start, and to manage critical elements of successful collaborations, including common ontologies, data ownership, and access. To tackle the urgent need for building data management systems that support data governance, provenance, semantics, curation, and assessment of quality, PCAST recommends that every NIH Institute and Center should appoint qualified data science officers to achieve this goal.

DOE Opportunities. The FY 2020 President's Budget for AI R&D within DOE is $162 million (not including the National Nuclear Security Administration). In 2019, DOE established the Artificial Intelligence and Technology Office (AITO) to coordinate AI-related projects and strategic AI technologies, both within the agency and with external partners in the domestic sectors and internationally. The AITO program office will also work to improve data management and to create an AI-enabled workforce.

The establishment of this coordination effort follows several recent DOE reports, ASCR Basic Research Needs for Scientific Machine Learning (2019),[24] Data and Models (2019),[25] and AI for Science (2020),[26] which identified key challenges and opportunities in methodologies, data, and scientific applications respectively. These reports identified opportunities for AI to benefit science, provided AI methodologies can be routinely integrated into science workflows.[27] PCAST recognizes this situation is similar to that at NIH in that large and increasing amounts of data are generated by DOE research, but these datasets generally are not AI-ready. Significant and rapid progress needs to be made to organize, harmonize, and integrate the activities outlined in the 2019 reports across DOE to realize the promise of AI to advance DOE-relevant science. PCAST expects this will require a substantial investment of resources and recommends DOE develop a 5-year and 10-year strategic plan as soon as possible to meet this critical challenge and to implement the opportunities identified in the recent DOE AI reports.

Recommendation 1.2: *Accelerate translational research in AI.*

To ensure U.S. leadership in translational AI, PCAST recommends a new strategic focus of research investments to grow translational R&D that puts emerging AI technologies into immediate practice to address specific impacts of COVID-19 as well as for other applications across U.S. industry and government. Specifically:

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[24] https://www.osti.gov/servlets/purl/1478744

[25] https://anl.app.box.com/s/f7m53y8beml6hs270h4yzh9l6cnmukph

[26] https://www.anl.gov/ai-for-science-report

[27] The DOE "AI for Science" report outlines opportunities in materials, environmental, life sciences, high energy, nuclear and plasma physics, as well as in engineering, instruments, and infrastructure. A central conclusion of this report is that the continued growth and expansion of DOE science infrastructures such as ESnet, new light sources, and exascale computation systems, is generating data at a scale and complexity that cannot be processed or even stored with current capabilities. This therefore demands AI-assisted design, operation, and optimization, for in-situ analysis of intermediate results, experiment steering, and instrument control systems. The DOE report gives examples in each of the above scientific areas that fall within its mission. Each discipline has its own specific needs, but the critical role of data generation, management and curation is essential to all areas.

Encourage all U.S. Federal agencies to elevate the importance of partnerships with industry to develop and deploy AI applications at scale, including applications such as intelligent citizen care and modernizing Federal data and information technology (IT) infrastructure, both of which have become increasingly urgent as a result of the COVID-19 crisis. These actions will drive new focused end-to-end R&D efforts in AI at a national scale and provide U.S. industry and the Federal Government with important world-class experience and expertise across the full lifecycle of AI applications. (I, G)

Create "AI Fellow-in-Residence" positions at NSF, the Defense Advanced Research Projects Agency (DARPA), NIH, NIST, DOE's AITO, and the General Services Administration's (GSA) Technology Transformation Services/JAIC AI Center of Excellence, with rotational opportunities for deep experts in industry and academia to share expertise, develop requirements, and more broadly influence strategic R&D directions for AI. (G)

- Encourage NSF to expand its partnership with industry to create a co-funded program that supports faculty and post-doctoral students working in AI to spend time in industry to better understand needs for AI technology and obtain continuous feedback for basic research. NSF also should allow graduate students supported through the Graduate Research Fellowship to spend time in industry as part of their educational experience.[28] (I, A, G)
- Universities should create a framework and incentives (accelerator funds, seed grants, industry-supported sabbatical leave) to support basic, application-driven, and interdisciplinary AI research and ease the process for rotational assignments across industry and academia. (I, A)

Pioneer and scale novel academia-industry AI partnership models**.** This will require a significant paradigm shift to university-corporate engagement strategies, effective agreements and intellectual property (IP) transfer vehicles (e.g., master agreements), willingness to embed industry partners on university campuses, allowing joint academia-industry appointments for faculty, etc. OSTP has convened an interagency roundtable, a national summit, and an NSTC Fast Track Action Committee to address these issues. Importantly, protection and confidentiality issues for industry data need to be addressed, a framework for on-site sabbaticals for faculty and post-doctoral students should be created, and researcher transitions between industry and academia (as well as industry and National Laboratories) should be addressed to remove disruptive implications of non-compete agreements in post-transition collaborations. (I, A)

Recommendation 1.3: *Create national AI testbeds.*

Deeper partnerships across industry, academia, and government will enable the United States to remain at the forefront of R&D in these key areas and well positioned to harness their value as new technologies and applications emerge. It is important to create a virtuous cycle aimed at the innovation infrastructure itself that can continuously accelerate R&D in AI. To create a pull for innovation and fuel R&D efforts in AI, the United States should develop national AI testbeds and define application targets for U.S. industry that allow it to create communities of discovery that accelerate efforts such as development of drugs and vaccines. The COVID-19 High-Performance Computing Consortium[29] and the CORD-19 dataset[30] are examples of the enormous value of creating platforms for sharing data and computational resources for accelerating efforts in S&T related to the crisis.

[28] The subcommittee envisions that such a partnership be co-funded by government and industry, with time spent in industry covered by industry funds.

[29] https://covid19-hpc-consortium.org

[30] https://www.whitehouse.gov/briefings-statements/call-action-tech-community-new-machine-readable-covid-19-dataset/

PCAST recommends the following actions:

Secure U.S. industry investment pledges to support core AI infrastructure. This would include grants to provide compute infrastructure for research and education related to AI (including free cloud credits and HPC cluster donations to universities, faculty, and students), open source AI frameworks, libraries and tools, contributions to advance U.S. leadership in AI R&D through open publications, and the creation of programs and joint laboratories and funding to support university and non-profit basic research on AI. (I)

Expand ongoing NSF-based programs to establish national AI research centers and infrastructure with sustained, long-term funding to enable cross-cutting research and technology transitions. These could include companion "mission-driven" AI laboratories that expand on the NSF AI Institutes program by providing facilities that allow AI researchers from academia, industry, and National Laboratories (see Section 2) to access unique data, tools, and expertise. These centers would enable research on core and applied AI (e.g., AI for agriculture, AI for manufacturing) as well as on cross-cutting topics such as AI for social good, the future of work, and harnessing big data. The centers could allow technology transition through partnerships between visiting fellows from academia, industry, and government labs, and will offer training for students at all levels. (G)

Direct the AI science mission at National Laboratories and across Federal agencies to drive the technical foundation for performing scientific research. National efforts in science should increase the use of AI technologies by developing intelligent research platforms and creating shared national resources, including data, computing, tools, and knowledge, that are made widely available to universities, National Laboratories, and industry for R&D. NIH, DOE and NSF should be tasked to develop new moonshot targets around topics such as accelerated discovery in science that drive advances in AI as well as the combination of AI, quantum, and HPC toward developing future paradigms for computing. Aiming at goals such as "creating 10 new critical materials and molecules for 10 industry sectors in 10 years" can be vital for driving innovation in AI and broadly advancing intrinsic capabilities in S&T. Investments should be made to upskill National Laboratories in AI (the United States currently lags behind Europe in AI publications).[31] (G)

Task Federal agencies such as NIST and NIH to curate, manage, and disseminate large data sets across critical areas for AI applications, working across U.S. agencies and with industry partners and other stakeholders. Data are the fuel for AI. NIST should continue to create a Test and Evaluation (T&E) foundation for AI that defines and implements standard evaluation methodologies and measures for AI systems and quantifies critical dimensions of performance for trustworthy AI including accuracy, fairness, robustness, explainability, and transparency. (G)

Recommendation 1.4: *Foster increased international collaboration in AI with key U.S. allies.*

Globalized access to information and accelerated technology disruption are collapsing the timescale for innovation in AI. Given the rapid pace of AI R&D worldwide, the United States should seek out, among its allies and like-minded partners, increased international collaborations with academic institutions and industry. This is critical for allowing the United States to stay ahead in the global AI race, particularly in working with other countries that are making significant investments and have strengths that complement U.S. capabilities.

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[31] Raymond, P., Shoham, Y., Brynjolfsson, E., Clark, J., Etchemendy, J., Grosz, B., Lyons, T., Manyika, J., Niebles, J.C. 2019. *Artificial Intelligence Index Report 2019*. AI Index Steering Committee, Human-Centered AI Institute, Stanford University, Stanford, CA. https://hai.stanford.edu/sites/default/files/ai_index_2019_report.pdf

PCAST recommends increasing international collaboration as follows:

Establish international partnerships in AI R&D with countries that share our values in the conduct of research, given compatible interests in AI technology and a strong pipeline of innovation and investments in AI at universities and industry in the respective countries.[32] Create a program for exchange of scientists across partner unions and nations to improve collaboration and information sharing in AI. (I, A, G)

Define joint international research programs in AI across the respective agencies—for example, by teaming NSF with corresponding agencies in the European Union to define research programs of joint interest in core and applied AI, as well as in the context of large centers such as NSF AI Institutes. Establish collaborative and reciprocal AI R&D centers across these unions and nations that include scientists and industry participants working jointly to advance critical topics in AI related to contextual AI, trustworthy AI, AI engineering, and AI hardware. (I, A, G)

Recommendation 1.5: *Attract and retain the best global talent in AI.*

PCAST finds it critically important that the United States remains a beacon for highly skilled talent. U.S. leadership in AI, and in many other areas of S&T—including QIS—benefits greatly from the contributions of its foreign-born residents and citizens. Ensuring continuity of this valuable component of the scientific workforce will be even more essential in the future of AI, as the science becomes more globally disseminated. It will be important to continue to provide training and work opportunities for suitably qualified individuals with a clear commitment to the United States and its values. (I, A, G)

Recommendation 1.6: *Establish an AI maturity model*.

The AI industry today is driven by a complex mix of optimism (given recent rapid advances with technologies such as deep learning) and growing realization that these approaches have fundamental limitations. On their own, AI technologies today are not sufficient to solve requirements for the AI component of IotF. New initiatives are needed to create trustworthy AI systems that advance AI capabilities and reduce the likelihood of adverse impacts. An overall AI maturity model is needed for U.S. industry that provides metrics for AI technologies and applications. Toward this goal, PCAST recommends the following:

NIST should take the lead working with other Federal agencies and industry to develop a maturity model for trustworthy AI that provides a framework for assessing and communicating the maturity and suitability of AI capabilities for deployment in the field, which could ultimately result in an AI accountability framework. This involves consulting nationwide with AI industry and academic researchers, as well as with stakeholders in basic research on trustworthy AI, such as NSF. This input should be used to build trust and understanding of mutual contributions to assure a successful partnership model and record best practices in the existing successful agreements. (I, A, G)

U.S. industry should become an active stakeholder in the creation of precision regulation to create trustworthy AI. Specifically, industry should convene stakeholders across government, industry, and academia to inform further development of the Federal Government's draft AI regulatory guidance[33] and to further build AI ethical frameworks and an AI maturity model that support innovation. Industry

[32] The Global Partnership in AI is a good example. https://www.state.gov/joint-statement-from-founding-members-of-the-global-partnership-on-artificial-intelligence/

[33] https://www.federalregister.gov/documents/2020/01/13/2020-00261/request-for-comments-on-a-draft-memorandum-to-the-heads-of-executive-departments-and-agencies

also should collaborate with the same to inform the development of open, consensus-based, globally recognized standards around trustworthy AI including fairness, ethics, accountability, reproducibility, and transparency. This includes leveraging the activities of appropriate multi-stakeholder organizations to create an agile framework for precision regulation of AI. (I, A, G)

Recommendation 1.7: *Drive opportunities for AI education and training.*

U.S. leadership in S&T for AI will require broadening the pool of potential AI scientists and engineers, and improving AI and related skills across the U.S. workforce. Increasing investment in STEM education will be more important and relevant than ever in the post-COVID-19 crisis world, given the growing requirements for data science, data management, curation and access, ML, and AI engineering.[34]

Toward this goal, the Federal Government should increase investments in national programs as follows:

Secure U.S. industry pledges to scale investments on training and education of the U.S. workforce in AI. This should include education and certification programs in AI, programs for reskilling workers in AI, and sponsoring research fellowships and residency programs in AI. Additional information about this recommendation can be found in the discussion and recommendations related to the third pillar, of ensuring a diverse and qualified IotF workforce, in Section 3 of this report. (I)

Develop AI curricula and performance metrics starting at K–12, and progressing through certificate/professional programs, and undergraduate and graduate courses. The development of curricula and educational materials should be coordinated among AI, computer science, and STEM pedagogy experts. Curricula should address emerging interdisciplinary AI areas, the societal applications and implications of AI, and highlight AI policy and ethical behaviors with regard to fairness, privacy, and data provenance. (A)

Engage secondary schools and universities to help train a highly skilled AI workforce at community colleges, and via certificate programs, online degrees, university programs, and workforce retraining programs. Develop incentives for careers in AI education together with training opportunities for teachers and educators and other professionals seeking retraining. Engage underrepresented and underserved populations to expand the talent pool and create outreach, diversity, and inclusion programs for AI (see Section 3). (A)

Create incentives, recruitment, and retention programs for AI faculty at universities, including research grants, graduate student scholarships, retention programs, and additional resources to support academic-industry partnerships (e.g., to enable easy access to special assignment or research leave for faculty who establish partnerships with AI industry). Also, promote faculty entrepreneurship and split appointments between academia and faculty-driven start-ups. Facilitate stronger alignment between faculty and industry by increasing faculty joint appointments with industry and industry appointments with universities, including industry engagement in curriculum development, teaching, and training. Employee contracts could be streamlined with non-compete requirements, and AI faculty workloads could be redefined, to enable faculty who are significantly engaged with industry (and may spend less time on campus) more flexibility to bring their invaluable industry-enriched educational perspectives to the classroom. Faculty partnering with industry face increased levels of expectations and their research agenda may shift toward the product needs and timeframes of the corporate partner. This may require allowing for flexibility of part-time positions over some period. Additionally, conflicts of interest must be disclosed and managed appropriately. (A)

[34] See also Section 3 of this report for complementary recommendations on *Meeting National Needs for a Diverse, Multi-Sector IotF Workforce*.

Increase NSF and Department of Education investments in AI educators, scientists, and technologists at all levels, specifically early career teachers and researchers, top students at universities, and post-doctoral fellows. This is important for developing the Nation's talent in AI and for ensuring they remain in the United States.

- Through increased funding levels, enable NSF to offer Graduate Research Fellowships for all U.S. undergraduate majors in computer science with GPAs above a certain threshold. Each year, more than 50,000 bachelor's degrees in computer science and related fields are awarded to U.S. citizens or permanent residents.[35] Each fellowship requires a commitment of ~$138,000 over 5 years (providing for 3 years of support).[36] (G)
- Support the Department of Education to develop a new national program for building AI skills digitally for an AI-ready workforce that empowers and enables students and mid-career professionals to realize the opportunity AI represents through continuous and tailored online training and education. (G)
- Task AI centers of excellence to advance skill development and learning in AI, including developing and sharing of educational content and facilitating outreach. Develop and share best practices for the most challenging problems of fielding successful AI systems, including establishing Federal databases for AI, curating and disseminating data, improving AI engineering practices, and achieving trustworthy AI in practice. (G)

Quantum Information Science

QIS includes the fields of quantum computing, quantum communications (and more generally quantum networking) and quantum sensing. Collectively, they represent the next frontier in the worlds of information processing and computation, secure communications, and novel navigation systems.

Background on Federal QIS Actions

The passage of the National Quantum Initiative Act[37] was a seminal moment for QIS, and a clear recognition of the critical importance of QIS in the security and prosperity of our Nation. As a sign of growing momentum, the President's FY 2021 Budget proposes a significant increase in QIS R&D and a commitment to double investment levels by 2022. If enacted, this would bring annual Federal spending for QIS R&D to more than $860 million by 2022.[38] It is worth noting that billion-dollar quantum R&D programs have been announced by (or across) China, the European Union, and India.[39]

The National Quantum Initiative Act aims to accelerate quantum R&D through increased spending, strengthened coordination of quantum R&D across the Federal Government, and new QIS consortia

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[35] https://www.nsf.gov/statistics/2018/nsb20181/report/sections/higher-education-in-science-and-engineering/undergraduate-education-enrollment-and-degrees-in-the-united-states

[36] National Science Foundation Graduate Research Fellowship Program Solicitation. https://www.nsf.gov/pubs/2019/nsf19590/nsf19590.htm

[37] National Quantum Initiative Act of 2018, Pub. L. No. 115-368 (2018). https://www.congress.gov/bill/115th-congress/house-bill/6227

[38] https://www.whitehouse.gov/wp-content/uploads/2018/09/National-Strategic-Overview-for-Quantum-Information-Science.pdf

[39] India ($1.06 billion): https://dst.gov.in/budget-2020-announces-rs-8000-cr-national-mission-quantum-technologies-applications; China ($1 billion since 2009): https://iopscience.iop.org/article/10.1088/2058-9565/ab4bea; European Union ($1.1 billion from 2018 to 2028): https://ec.europa.eu/digital-single-market/en/policies/quantum-technologies-flagship

around the country.[40] In response to this legislation, The White House established the National Quantum Coordination Office to coordinate Federal R&D efforts. NSF and DOE are establishing QIS Centers; NSF is reviewing proposals for Quantum Leap Challenge Institutes; and DOE has released a Funding Opportunity Announcement for larger QIS Centers. In addition, NSF and DOE—through a formal agreement—are working to ensure a coordinated review and implementation of the new QIS Centers.

Recommendations

PCAST identifies actions below that can be taken to accelerate U.S. quantum leadership. Sectors that would take principal responsibility are indicated as follows: I = industry, A = academia, and G = government.

Recommendation 1.8: ***Engage industry in building world-class quantum infrastructure at scale. (I)***

The United States should lead the world in creating and applying quantum computing systems, centers, and services. It is estimated that industry will invest more than $2 billion between 2020–2025 to design, build, and deploy high-availability quantum computing systems, execute a roadmap that will at least double system performance every year, and build cloud-accessible quantum computational centers and associated services.

Recommendation 1.9: ***Invest $100 million annually over 5 years to create federally funded national quantum computing user facilities. (G)***

Establish national quantum computing user facilities to jump-start quantum algorithm and application development and quantum computer science, make available a critical scientific and computational resource to scientists at U.S. National Laboratories and universities, and serve as a market-making catalyst to accelerate the growth of U.S. industry producing quantum hardware and software. PCAST recommends a Federal investment of $100 million/year for the next 5 years to create quantum computing user facilities leveraging the output of the multi-billion-dollar investments that industry is undertaking designing and building quantum computing systems.

This approach is akin to the HPC user facilities DOE and NSF have successfully sponsored and deployed for many decades. Such facilities, among many other use cases, have become foundational in the fight against the coronavirus as part of the COVID-19 HPC Consortium. Quantum computing user facilities will undoubtedly become equally essential for a broad range of research needs of the U.S. R&D enterprise in this decade. We highlight that specific use cases for quantum technologies across the U.S. Government are being explored by the End-User Working Group of the NSTC Subcommittee on Quantum Information Science (SCQIS).

Recommendation 1.10: ***Lead the world in the creation of a quantum internet and intranet. (I, A, G)***

The creation of the Advanced Research Projects Agency Network (ARPANET), which resulted in today's internet, is a model for the establishment of a quantum internet and intranet. A quantum network would provide a testbed for developing required components, such as qubit transducers and quantum repeaters, and a mechanism to explore quantum network protocols, cryptography, and applications for distributed quantum entanglement under the National Quantum Initiative Act scientific effort. This work would exploit synergies between quantum computing and quantum communication. Linking these two fields early could enable researchers to demonstrate remote entanglement technologies and

[40] National Quantum Initiative Act of 2018, Pub. L. No. 115-368 (2018).

protocols for secure quantum sensing, communication networks, and secure quantum cloud computing. We highlight the National Quantum Coordination Office report from February 2020, *A Strategic Vision for America's Quantum Networks*, as containing specific pathways to achieving these goals.

Recommendation 1.11: ***Attract and retain the best global talent in Quantum Information Science and Technology. (I, A, G)***

As was highlighted for AI, PCAST also recommends a renewed emphasis on attracting and retaining highly skilled foreign students, scientists, and engineers in QIS to enable the U.S. effort to continue to benefit from the best global talent.

The Role of Academia in Quantum Information Science

Many of the intellectual drivers for QIS have come from academia, where exploration of the boundaries of conventional disciplines and expansion of intellectual frontiers are essential mandates. Universities provide top-level intellectual capability for applications and foundations of QIS and technologies.

In addition to research in the academic setting, which is typically limited to relatively small consortia, university researchers can collaborate creatively in partnerships with industry and government to accelerate the development of quantum information processing in all aspects. Universities are uniquely positioned to lead new forms of partnership in QIS. Thus, universities can act as the pivot point for partnerships supported by private foundations and industrial partners, in which academic researchers may work together in focused efforts targeting foundational and long-range research in QIS.

Another strength of academia is the ability to collaborate and share scientific progress internationally. Although collaboration and sharing are basic characteristics of academic research, universities can build on them to create *Open Frontiers Discovery Teams* composed of small-scale discovery-based partnerships between U.S. universities and selected foreign university partners, enabling groups of 3–10 academic scientists to explore fundamental research in selected topics.

Lastly, academia has a key role to play in educating the next generation of scientists and citizens, which PCAST refers to as *the quantum generation*. New modes of teaching are needed for a new science that is characterized by the unusually large extent of interdisciplinary work that characterizes QIS. Here, universities can work to develop innovative teaching partnerships among disparate disciplines within academia, between academia and industry, and between academia and National Laboratories, to create flexible curricula and industry-infused shared education modules. This will require new modalities for appointments and leaves-of-absence in all three sectors, to enable teaching or co-teaching across both traditional disciplinary boundaries and the conventional boundaries between academia, industry, and National Laboratories. Universities also can partner with industry and National Laboratories to develop a broad, needs-focused quantum education at the pre-college and post-college levels.

Recommendation 1.12: ***Foster discovery-based science across all sectors. (I, A, G)***

Academia has a critical role to play in expanding and exploring the frontiers of QIS and related technology, and in building top-level intellectual capacity at the boundaries of foundational and applied research. Universities provide strengths that are complementary to those of industry and National Laboratories. They should not compete with these other two sectors but instead, in addition to individual efforts, collaborate in larger partnerships with the other sectors.

Recommendation 1.13: ***Provide curated access to quantum technologies. (I, A, G)***

Establish Strategic Quantum Access—a three-way alliance among industry, government laboratories, and universities to speed development of practical quantum computing applications. This is inspired by the successful HPC strategy. For quantum computing, PCAST envisions industry supplying hardware to government laboratories which can be used to drive quantum computer science and application research. As with HPC, this hardware would constitute a set of national quantum computing user facilities providing access to quantum computation for all three sectors.

Alongside these efforts, relevant Federal agencies could develop competitive programs for university-led research into fundamental issues underlying quantum information processing (quantum complexity theory, algorithms, applications, new materials, and other headlight research). These programs would have focused goals and make use of the talent in academia to improve and accelerate the development of new materials and qubit devices, as well as quantum computer science and applications through the industry and National Laboratories partnership program.

Recommendation 1.14: ***Create a pre-competitive quantum research collaboration (QRC). (I, A)***

For example, companies could combine efforts to support a group of researchers at multiple institutions, observing and leveraging research to influence long-term development of hardware. Models for this currently exist in the data science area, some with NSF seed funding. A successful model for this is the Semiconductor Research Corporation (SRC). PCAST envisions 5-year programs, with the recently established Quantum Economic Development Consortium (QED-C) a promising pathway to achieve this objective.

Recommendation 1.15: ***Create foundational discovery institutes.***

Foundational discovery institutes would provide long-term funding for teams of faculty members to work together in focused efforts, targeting crucial issues relevant to quantum technologies: new materials, devices, algorithms, and applications. Longer programs over 15–20 years are envisioned. An existing model deserving longer-term support is the NSF Quantum Leap Challenges Institutes (QLCI). The Joint Services Electronics Program (JSEP) is also an early prototype of a discovery institute that made a significant impact. (A, G)

Another model is university-based institutes of quantum researchers funded by private foundations—facilitated or co-funded by NSF or other appropriate agencies—that collaborate with industrial partners. Researchers in these institutes could work together in focused efforts targeting foundational and blue sky research in quantum science over 5 to 20-year horizons. An example of one such (international) model is QuTech in Delft, Holland (which includes the Kavli Foundation, TU Delft, quantum industrial partners, and the Netherlands Organization for Applied Scientific Research).[41] (I, A, G, Foundations)

Recommendation 1.16: ***Educate a quantum-enabled workforce. (I, A, G)***

One of the major challenges to building a critical capacity of talent in QIS is that U.S. universities as a whole do not have curricula in place to train the next generation of specialists in these fields. By leveraging public-private partnerships, institutions of higher education across the United States can create novel curricula and training programs to spark undergraduates, graduate students, post-doctoral fellows, educators, and faculty interest and advance QIS education. In addition, educational programs designed with industry-recognized, skills-based credentials in mind (as discussed in Section

[41] https://qutech.nl/

3) could give students confidence that their degrees are preparing them to succeed in the jobs of tomorrow.[42]

Opportunities for industry to accelerate QIS education (I)

The United States should lead the world in the creation and delivery of industry-relevant quantum educational and training programs, with the goal of reaching **10 million interactions by quantum pioneers between 2020 and 2025.** Industry can play a major role in this endeavor. Investments can range from open access to quantum technology systems and services to developing and sharing open source quantum software communities and open quantum curriculum, including quantum textbooks, YouTube channels, and lecture series. Investments also should be made in educational enrichment events, including sponsoring workshops and conferences, supporting QIS academic programs, work-based learning opportunities, industry internships and post-doctoral programs, certification programs, quantum science and engineering hiring programs, and expanded representation of women and minorities within the QIS field.

Workforce development and training through collaborative partnerships (I, A, G)

PCAST also recommends Federal funding agencies grow their support for joint university-industry graduate student research—such as the NSF Quantum Information Science and Engineering Network (QISE-Net) program—and broaden the scope to include quantum engineering and computer science. In addition, PCAST recommends the creation of quantum programs that cater to high school and undergraduate students.[43] Innovative teaching partnerships should also be established among disparate disciplines both within and across academia, industry, and National Laboratories. New internal hiring structures could be introduced to allow appointments of scientists from industry and the National Laboratories as co-instructors for courses in quantum science and technology at colleges and universities. Teaching across traditional disciplinary boundaries would help to accelerate learning and remove barriers among relevant science, computing, and engineering disciplines. NSF QLCI could also be leveraged to promote the development of cross-disciplinary training, and other NSF initiatives could drive diversity and inclusion in the quantum workforce, especially through engagement at pre-college levels (such as Innovative Technology Experiences for Students and Teachers, or ITEST). Partnerships with industry and National Laboratories could be leveraged to design and introduce broad needs-focused quantum-related programs and curricula for the pre-college level and professional certification levels.

Finally, an area for further consideration beyond highly specialized QIS R&D fields is building a skilled technical workforce in related areas of importance, for example, through continuing education, reskilling, and retraining opportunities. Further discussion of such opportunities may be found in Section 3 of this report.

Recommendation 1.17: ***Build international R&D collaborations at the frontiers of QIS. (A)***

PCAST also recommends building small-scale discovery-based partnerships between U.S. universities and selected foreign university partners. Such partnerships should enable teams of 3–10 academic

[42] This section is intended to complement the recommendations for *Meeting National Needs for a Diverse, Multi-Sector IotF Workforce* contained in Section 3 of this report.

[43] See "Quantum Computing as a High School Module" as an excellent example of new content catered for high-school students. See also Key Concepts for Future Quantum Information Science Learners at https://qis-learners.research.illinois.edu/

investigators to explore fundamental research in selected topics of mutual benefit. Academic members of the teams could each connect locally to industry partners.

Recommendation 1.18: ***Foster national security by sharing guidance with universities. (A, G)***

The NSTC Subcommittee on Economic and Security Implications of Quantum Science (ESIX) is tasked with maintaining approaches for fostering national security while enabling scientific development and economic growth. PCAST recommends this committee assist academic researchers and universities by continuously evaluating the security implications of QIS and providing guidance to universities about research opportunities and how best to navigate the boundary between open and classified research.

Accelerated Discovery Powered by the Convergence of HPC, AI, and Quantum Computing

Discovery lies at the heart of every scientific endeavor, and discovery or fundamental research is the foundation driving the creation of new technologies, new ideas, and deeper insights. The COVID-19 pandemic highlights the importance of scientific discovery for the design of new medicines, vaccines, and pharmaceutical products.

However, in the past, discovery—which fuels both incremental and breakthrough advances in many fields—has in many cases been serendipitous or alternatively a slow and iterative process between computer-assisted simulations and experimental testing. Continuous advances in HPC have helped accelerate discovery, for example by reducing vast libraries of potentially useful molecules to a much smaller set of probable leads for therapeutically active compounds. Ever-more powerful computational software is helping simulate molecular interactions for more targeted cancer immunotherapy, leading to better catalysts for creating high-performance plastics, and creating more durable electrolytes for high-energy-density batteries for electrical transport.

In the current pandemic, the COVID-19 HPC Consortium is providing researchers with access to over 485 petaflops (485 thousand million million floating point operations per second) of heterogenous computational infrastructure—spanning government, industry, and academia—for running very large numbers of calculations in epidemiology, bioinformatics, and molecular modeling to advance the pace of scientific discovery. This offers great promise for accelerating the development of new treatments and the discovery of a cure.[44] Nonetheless, the discovery and design process of small molecules for drugs or industrial materials remains a lengthy and costly endeavor in both human expertise and computational power.

Two additional computing approaches—quantum computing and AI—have the potential to reshape discovery by complementing the strength of classical HPC while addressing its shortcomings.

Although quantum computers are still at the dawn of their innovation journey, the potential for accurate simulations of chemical reactions is real. Molecular simulation requires mimicking the interactions between electrons in each atom with the nuclei of all other atoms. The bigger and more complex a molecule is, the more difficult this process becomes. Today's supercomputers can simulate relatively simple molecules, but when researchers try to develop new complex compounds—whether for life-saving drugs or better batteries—classical computers cannot achieve the same accuracy, and may not be able to carry out a simulation at all.

In contrast, as far back as 1981, Nobel Prize–winning physicist Richard Feynman predicted that computers based on quantum mechanics could simulate large molecules exactly, rather than only

[44] https://covid19-hpc-consortium.org/

approximately. Today, researchers are working to apply this emerging technology for solving real world problems. It Is anticipated that quantum computers will outperform any classical computer—even if all classical computers were combined together—in certain use cases such as quantum chemistry.

As quantum computing addresses the accuracy limits of classical HPC simulations for solving chemistry problems, AI can play a crucial role in efficiently and constructively exploring the vast chemical search space—and already is making a mark on the process of discovery. Leveraging past simulation and experimental results, researchers are training sophisticated deep learning models to predict molecular interactions and subsequent drug or material properties based on molecular compositions and synthesis processes. In addition, generative AI models support the creative portion of identifying material compositions to yield desired properties.

For example, generative AI models have recently identified 3,000 small molecules as candidates for binding to the Viral S-protein of SARS-CoV-2.[45] In addition, AI plays an important role in structuring data that feed such powerful models. In 2018, some 450,000 new papers were published in the field of materials science alone. In March 2020, government, industry, and academia worked together to release the COVID-19 Open Research Dataset, known as CORD-19, with nearly 130,000 scientific articles about the SARS-CoV-2 virus (as of June 28, 2020) as well as related viruses in the broader coronavirus group.[46] A staggering amount of data and knowledge is buried in that textual representation. Thanks to AI, it is now possible to derive more information than ever from these data resources; AI systems are already helping researchers sift through and sort vast scientific and technical literature to accelerate research. However, to enable the full potential of AI for scientific discovery, it is essential that the data be generated and stored in modes accessible to AI analysis.

As powerful as each of the three computing methods is at supporting the quest for new drugs and materials, the S&T ecosystem has not yet fully grasped the future potential at the convergence of *Bits + Neurons + Qubits* for solving problems that previously were thought unsolvable. And it is not simply the increased computational capability wrought by joining the elements above that will enable a dramatic acceleration of discovery, but instead their combination in complex scientific workflows.

Today, scientific methodology is still largely grounded in the big-data approaches that are heuristics-based, human expert-driven, and largely linear. However, PCAST believes that AI—together with leaps in classical and quantum compute power—has the potential to transform science by enabling deeper capabilities for knowledge extraction and representation, the development of closed-loop methods for automated hypothesis generation and testing, and realization of self-driving labs that automate high-throughput experimentation to bridge digital models and physical testing.

Figure 1 shows the **Accelerated Discovery Workflow** of the future. It is composed of four steps. *Deep Search* (step A) leverages AI to derive information and data from the collective domain knowledge stored in documents such as scientific publications and lab reports. *Intelligent Simulation* (step B) augments the known with classical or quantum simulations optimized to yield maximum information gain. AI *Generative Models* (step C), trained on the aggregate data from steps A and B, identify new ideas and possibilities (such as the chemical composition and structure of candidate molecules for desired physical or chemical properties such as binding energies necessary to inhibit proteins of viruses). *AI-*

[45] Chenthamarakshan, V., Das, P., Padhi, I., Strobelt, H., Lim, K.W., Hoover, B., Hoffman, S.C., and Mojsilovic, A. 2020. "Target-Specific and Selective Drug Design for COVID-19 Using Deep Generative Models." arXiv:2004.01215v1 [*cs.LG*] 2 Apr 2020; https://arxiv.org/pdf/2004.01215v1.pdf

[46] https://www.semanticscholar.org/cord19

Driven Experimentation (step D) AI accelerates experimentation by performing *in-situ* analysis during the experiments and using this analysis for real-time control of experimental parameters in labs.

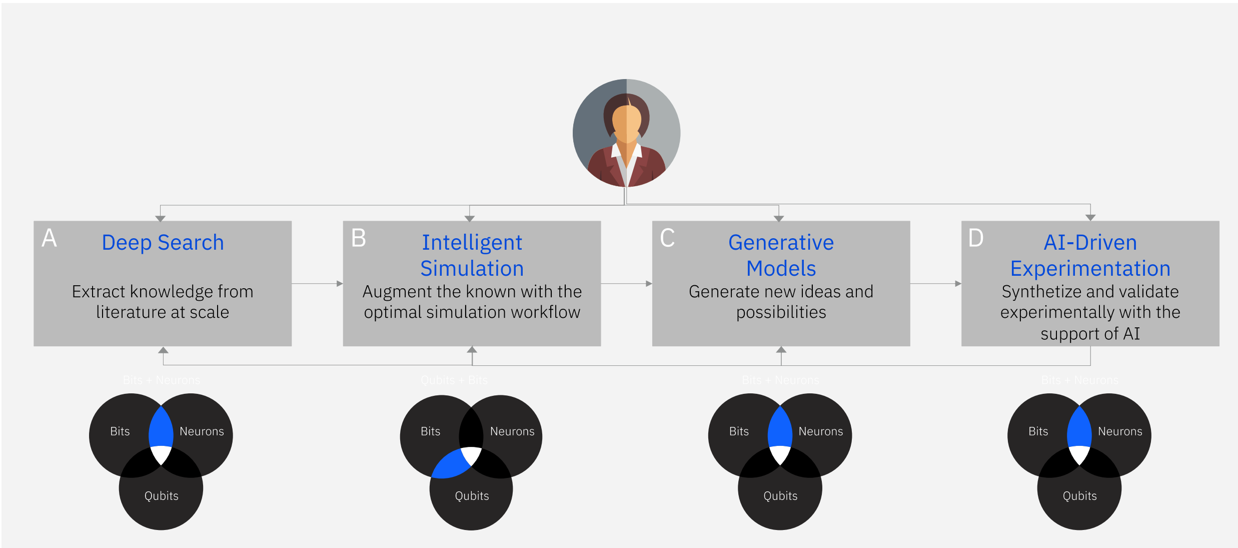

Figure 1. Accelerated Discovery Workflow

Following this workflow should enhance the productivity of scientists and engineers involved in the process of discovery. They will play a key role in each step—curating the data AI will extract from the literature to increase its relevance, influencing the selection of the computational method, contributing their own creativity to the designs proposed by the AI generative models, and selecting the overall scale of the AI-driven experimentation process. When brought together, PCAST believes that a tenfold acceleration in discovery will become possible.

The Accelerated Discovery Workflow can be broadly applied to a range of scientific endeavors. For example, it is currently estimated that without fast-tracking, at least 10 years and $2.6 billion are required to develop one new medicine including the cost of many failures. Only 12% of compounds that enter clinical testing receive FDA approval.[47] The most common reasons for failure are either a lack of understanding of the mechanism of action (wrong target) or off-target effects (toxicity). The use of massive AI and HPC capabilities can help identify new targets by analyzing the large amounts of biological data being generated through new technologies like single cell RNA sequencing. These technologies allow researchers to identify the genomic and transcriptomic drivers of behaviors of individual cells in tissues. Identification of novel targets, then screening large libraries of compounds that can modify those targets, is already underway and has been critical for driving the development of vaccines for COVID-19.

However, accelerating drug discovery, and improving the accuracy of target identification, mechanism of action, and potential off-target effects can supercharge drug discovery and dramatically shorten timelines from the bench to the clinic. These factors also can vastly reduce the cost of drug development, improve therapeutic outcomes, lower health care costs, and utilize data-driven

[47] DiMasi, J.A., Grabowski, H.G., and Hansen, R.W. 2016. “Innovation in the pharmaceutical industry: New estimates of R&D costs.” *Journal of Health Economics* 47:20-33.

approaches to implement and individualize therapies. The implications on healthcare from successful combination of AI and quantum-powered drug discovery are hard to overestimate.

Additional potential applications with significant economic impact PCAST believes would benefit from the convergence of HPC, AI, and quantum computing include metamorphic manufacturing; financial technology (FinTech), such as algorithmic trading; marketing by aggregating huge volumes of data to influence consumer decisions and spending precisely; meteorology through improved pattern recognition and processing speed for weather prediction; and logistics through optimization of workflows associated with transport management, fleet operations, traffic control and supply chain management. In many cases, issues of data security, privacy, and propriety exist and need to be addressed.

Recommendation 1.19: ***Expand and redefine the mission of the National Strategic Computing Initiative (NSCI). (G)***

The National Strategic Computing Initiative (NSCI)[48] was launched by Executive Order 13702 in July 2015 to advance U.S. leadership in HPC. The NSCI is a whole-of-Nation effort designed to create a cohesive, multi-agency strategic vision and Federal investment strategy, executed in collaboration with industry and academia, to maximize the benefits of HPC for the United States. Due to the prohibitive nature of continuing to scale classical silicon technology, it will become necessary, after exascale (computing systems capable of at least a quintillion calculations per second), to fundamentally redefine how systems are designed and built to deliver U.S. leadership in computing.

In November 2019, the NSTC Fast Track Action Committee on Strategic Computing released the report *Updating the Nation's Strategic Approach to Computing*. PCAST supports implementing the recommendations of that report and further recommends that a new Executive order be issued to expand the mission of the NSCI to ensure that the United States is the undisputed leader in both HPC and a new generation of scalable systems designed to seamlessly integrate complex heterogeneous technologies (combining high-precision cores and AI accelerators), together with fundamentally different computing architectures such as quantum computing.

To contextualize this opportunity, consider that within the next 3–5 years it is quite likely that it will be possible to create:

- High-precision classical processors with more than 30 billion 5+ GHz transistors (bits);
- Neural processors with more than 100 TOPS (tera operations per second) per Watt for training and more than 500 TOPS/Watt for inferencing (artificial neurons); and
- Quantum processors with >1,000 qubits and 100x lower error rates than today's state of the art (qubits).

As impressive as these capabilities are, their most profound implications are in creating a new generation of systems and workflows to take advantage of the combined capabilities of these three information processing architectures.

PCAST recommends that the NSCI be expanded to add significant focus on the development, delivery, and use of advanced computing technologies by a broad spectrum of commercial and research enterprises. Additionally, a major focus should be placed on embedding AI throughout the applications,

[48] https://www.whitehouse.gov/wp-content/uploads/2019/11/National-Strategic-Computing-Initiative-Update-2019.pdf

as well as in the software running the system and in the datacenter. Most computing in the future will be delivered via the cloud, and the massive investments in that space should be leveraged.

PCAST further recommends a stronger emphasis on the importance of addressing software challenges, including complexity, correctness, trust, and sustainability. The usability and enablement of advanced computing for those without deep supercomputing skills should be equally prioritized. It is important to recognize that future computing initiatives should focus directly on scientific, economic, and societal impact, rather than on simply building systems with increased peak performance.

Recommendation 1.20: ***Pilot the Accelerated Discovery Workflow in the newly proposed IotF Institutes. (G)***

The new IotF Institutes recommended as the cornerstone of the second pillar (described in Section 2) of this report) are a natural venue to test the implementation and practice of the proposed Accelerated Discovery Workflow. Another opportunity to apply this approach is in the materials science domain, illustrated through specific recommendations for a data-intensive DOE initiative described below.

Recommendation 1.21: ***Re-energize and scale up the Materials Genome Initiative (MGI).***

The MGI is a Federal Government, multi-stakeholder initiative to develop an infrastructure to accelerate and sustain domestic materials discovery and deployment in the United States. A 2018 NIST-commissioned report[49] estimates the potential economic benefit of an improved materials innovation infrastructure for the United States to be between $123 billion and $270 billion per year. PCAST therefore recommends the following actions:

Place AI and quantum at the heart of the MGI by pioneering the emerging Accelerated Discovery Workflow. (I, A, G)

Define a set of Materials Grand Challenges. (I, A, G)

Commission an appropriate group of experts to define the most important materials to pursue for U.S. success across a broad array of sectors (e.g., vaccine discovery, fertilizers in agriculture, and new lithium chemistry batteries for electric transportation). Define three categories: top-5 materials to discover in the next 5 years, top-10 in the next 10 years, and top-20 in the next 20 years.

Launch DARPA-style competitions and large prizes for the Materials Grand Challenges. (I, G, Foundations)

Scale investments in software engineering and computational capacity in the U.S. National Laboratories to support the Accelerated Discovery mission. (I, A, G)

Consistent with these recommendations, PCAST also recommends in Section 2 of this report creating a unique set of IotF Institutes that integrate multiple IotF fields to tackle foremost problems of societal importance, leveraging the capabilities of America's DOE National Laboratory system.

[49] https://www.nist.gov/system/files/documents/2018/06/26/mgi_econ_analysis.pdf

2. New Models of Engagement for National Laboratories

One of the crown jewels of America's multi-sector research enterprise (private industry, academia, government, and non-profit organizations) is the system of 17 U.S. DOE National Laboratories.[50] Emerging after World War II, these laboratories span a huge range of topics in research and development—from clean energy to particle physics to human health, materials science, and biology. These highly successful organizations, which operate world-class facilities and house some of the most successful researchers on the planet, represent a unique opportunity to implement new approaches to multi-sector R&D partnerships. In so doing, they facilitate leveraging the strengths of each R&D sector and obtain a multiplicative factor of effectiveness that cannot be achieved in other ways. Many of the laboratories already are playing significant roles in IotF. In this section, PCAST proposes a new model of partnerships enabled via the National Laboratories, identifying key actions and engagement across industry (I), academia (A), and government (G).

A New Framework for Multi-Sector Partnerships: IotF Institutes

As noted in Section 1, extraordinary opportunity exists for America to continue leading the world in IotF. One particular strength in that leadership involves strategically combining two or more of those areas on compelling problems of societal importance. Toward that end, PCAST proposes the formation of IotF Institutes—a new class of multi-sector institute offering innovative frameworks for R&D partnerships among government, industry, academia, and non-profit S&T organizations. Specific recommendations follow.

Recommendation 2.1: ***The Federal Government should establish policies and frameworks for IotF Institutes, (G)*** *emphasizing:*

- Research portfolios of collaborative projects at the intersection of two or more IotF areas—ranging from fundamental research to the applied demonstration of technology—that complement established federally supported programs;
- IP terms that incentivize participation and innovation from industry, National Laboratories, academia, and non-profits to drive commercialization of IotF technologies at scale;
- Administrative structures that reduce unnecessary regulatory burdens and maximize productivity and innovation while maintaining appropriate transparency and accountability; and
- Physical locations that serve as regional hubs for technological, economic, and skill development, leveraging Opportunity Zones, HUBZones, and other incentive structures.

The IotF Institutes will expand upon a strong existing national foundation by implementing new models to accelerate the delivery of S&T advances and by introducing improvements to increase return on investment and drive commercialization of technology at scale. With these Institutes, America will transcend and leverage the past, not seek to recreate it. At the same time, past bastions of S&T excellence, such as Bell Laboratories, have been lost to a world where the risks and complexities of blue sky research, globalization, and paths to market created challenges no one entity could overcome for delivering the required advancements and innovations that will underlie American competitiveness in IotF. The newly proposed approach will help to overcome these challenges. The result will be an adaptable, flexible new model built to let all parts of the U.S. S&T infrastructure work together seamlessly.

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[50] The National Laboratories comprise the DOE National Laboratory complex, consisting of 17 independent organizations. Ten of those, managed under the DOE Office of Science, are the focus of program proposed herein.

Basic and applied research are both required to realize this vision: better integration of basic and applied initiatives will improve the transfer of fundamental discoveries to commercial markets. New modes of engagement will be embraced, leveraging the best of government, industrial, academic, and non-profit institutions. Unnecessary and ineffective administrative burdens will be reduced or eliminated, addressing IP challenges and opening the door for exploration of new ideas, especially those having high intellectual risk but potentially enormous societal benefit. Tight coupling between fundamental and applied research will also enable rapid feedback and improve deployment. The past, and the strong foundation it built, provides a launch pad for this new approach—one sure to maintain and improve American S&T superiority.

Although the five IotF areas should continue to advance independently through efforts such as those launched under the American Artificial Intelligence Initiative[51] and National Quantum Initiative Act,[52] an extraordinary opportunity lies in applying several of the five IotF areas in a cross disciplinary manner, in order to solve grand challenge imperatives of societal significance. Accordingly, the IotF Institutes will aim to leverage this convergence through multi-sector partnerships, partner-favorable IP policies, tax incentives to accelerate economic growth, the formation of a competitive ecosystem to increase the pool of talented researchers in IotF, and close cooperation between basic and applied research endeavors to maximize intellectual interactions for a virtuous cycle of innovation. With a confluence of world-leading researchers from different disciplines spurring an acceleration of unanticipated discoveries having practical end goals in mind—much like the structure of the celebrated Bell Laboratories—the IotF Institutes will be unique, transformative environments that both accelerate the pace of fundamental research and yield pathways toward new products and services.

DOE's National Laboratories will play a vital role in realizing the IotF Institutes and shaping their underlying frameworks. Figure 2 illustrates a range of opportunities for engagement in the IotF Institutes for all Federal and National Laboratories. Although the established mission and expertise of a particular laboratory group relates to the role it may play in advancing an individual IotF area, the inherently integrated nature of the proposed IotF Institutes and their potential to amplify one another (e.g., QIS empowering advances in biotechnology) enables each distinct intersection to yield dividends for the others and enhance discoveries in a feedback cycle.

For instance, the proposed expansion of biotechnology capabilities within the IotF Biotechnology Institute (one of the first two proposed flagship Institutes) will support the development and impact of all IotF at NIH and U.S. Department of Agriculture (USDA) Laboratories. Similar advances in other IotF Institutes are anticipated to enable discovery in advanced manufacturing technologies such as digital twins and additive manufacturing (3D printing).

[51] https://www.whitehouse.gov/ai/

[52] https://www.congress.gov/bill/115th-congress/house-bill/6227

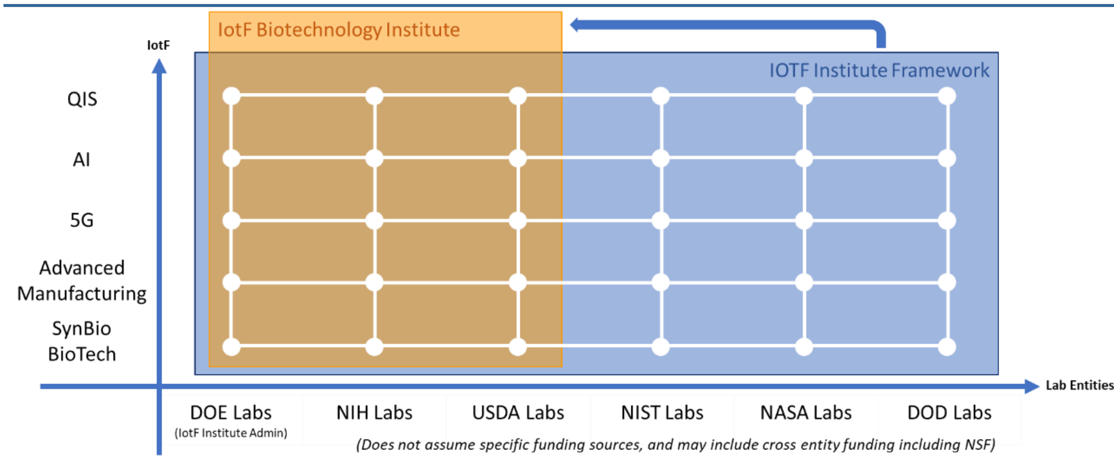

Figure 2. Anticipated breadth of engagement and collaboration for Industries of the Future Institutes.

The IotF Institutes are intended to have a substantial positive impact upon fundamental and applied aspects of advanced scientific research across all R&D sectors of academia, non-profits, National/Federal Laboratories, start-up companies, and established industrial leaders. Furthermore, they address critical themes that underlie our Nation's competitive advantage. The IotF Institutes would present a new means of catalyzing world-shaping research; foster cross-agency and industry partnerships; maximize time for research (at National Laboratories in particular) by reducing unnecessary bureaucracy; facilitate a business-friendly IP framework that encourages investment; establish world-class multi-user facilities that likewise support the Workforce of the Future; strengthen the pipeline for the technical talent pool; and develop world-class personnel with access to stable funding streams—all of which lead to a positive and sustainable national economic impact. Some of these aspects are known gaps today, and it is intended that the IotF Institutes address these gaps in the interest of our Nation's competitive advantage.

The proposed IotF Institutes should also aggressively develop domestic talent from across our Nation's demographic spectrum, while concurrently attracting the best and brightest researchers in the world to the United States for pursuit of advanced degrees and subsequent U.S. employment and contributions in IotF fields. The DOE is envisioned as the steward for the IotF Institutes, and budget and resources should be appropriated to facilitate both talent acquisition and associated capability development. Furthermore, compensation, hiring, and retention of talent within the IotF Institutes will require special consideration (see Section 1). Academia, industry, and National Laboratories utilize distinct compensation models for technical staff. Differences among these models will be revealed in multi-entity collaborative initiatives such as the IotF Institutes proposed here. Compensation and benefits are only one facet of a researcher's employee experience, however. Progressive compensation strategies should be proactively developed and deployed by IotF Institute administration to assure continued talent balance across our Nation's S&T enterprise. Finally, these recommendations should be pursued in a manner that preserves momentum on programs with established value; the intention is not to reinvent the wheel, but rather to assure alignment of purpose and maximum impact in the interest of our Nation.

Key Attributes of the IotF Institutes

The pace of technology continues to accelerate, and therefore solutions are needed that can address near-term challenges while simultaneously laying the groundwork for the future. To that end, IotF Institutes that will serve as inclusive and innovative environments are proposed to explore the impact and intersection of IotF. The Institutes are intended to cultivate scientific creativity and technical talent—bringing the best minds and tools together in one entity to significantly accelerate IotF in the United States. It is intended that the proposed IotF Institutes provide greater flexibility for public-private partnerships compared with previous models to facilitate transfer of technology from the laboratory to large-scale production, enabling a high return on investment for all participants.[53]

Recommendation 2.2: ***IotF proposals should engage partners from all sectors. (I, A, G)***

This includes industrial partners who can support large-scale translation of discoveries to products, as well as leading researchers across the government, academic, and non-profit spectrum.

The IotF Institutes could be initiated by DOE through a competitive process to serve as S&T collaboration zones driven by public-private partnerships and projects. These collaboration zones will accelerate national as well as regional economic development, diversify our concentrated areas of technology development, and accelerate the development of a highly capable STEM workforce.

Recommendation 2.3: ***IotF Institutes should be distinct from but complementary to established institutes, initiatives, and National and Federal Laboratory activities. (G)***

The proposed IotF Institutes should readily leverage and contribute to the output of existing institutes and initiatives.

The proposed IotF Institutes are intended to complement existing efforts within our National and Federal Labs by extending beyond fundamental research and development in IotF to demonstration and validation of IotF technology-based solutions to current and emerging challenges. They would be positioned to leverage and amplify key National Laboratory resources. For example, they could work with the recently established DOE AITO to gain visibility for industrially relevant technologies, and to find and cultivate technologies through at-scale demonstrations in the Institutes.

Recommendation 2.4: ***IotF Institutes should establish transparent IP terms that promote investment by partners and enable commercialization at scale. (I, A, G)***

To facilitate efficient development, adoption, and scaling of novel technologies, PCAST proposes that participation and IP agreements be assessed and refined for IotF Institutes. While some elements of an effective IP framework have been proposed, for example in the Manufacturing USA Framework,[54] the extent to which these guidelines have been implemented in practice is unclear, and industry representatives have suggested that additional refinement is warranted.[55] Separately, a recent review of the National Nanotechnology Initiative conducted by the National Academies of Sciences, Engineering, and Medicine suggests that large-scale commercialization of nanotechnologies in the United States is being outpaced by that of other countries. The authors recommended strengthening the lab-to-market innovation ecosystem to enable translation of research to products. While this

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[53] NIST. 2019. *Return on Investment Initiative, To Advance the President's Management Agenda*, Final Green Paper, April 2019. https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.1234.pdf, accessed June 4, 2020.

[54] Guidance on Intellectual Property Rights for the National Network for Manufacturing Innovation, 2014. https://www.manufacturing.gov/sites/default/files/2018-01/nnmi_ip.pdf

[55] National Academies of Sciences, Engineering, and Medicine. 2019. *Strategic Long-Term Participation by DoD in Its Manufacturing USA Institutes: Proceedings of a Workshop*. Washington, DC: The National Academies Press. https://doi.org/10.17226/25440

problem is multifaceted, the report highlights the value of flexible IP terms in public-private partnerships for accelerating commercialization.[56]

PCAST proposes that the IotF Institutes provide clarity of IP terms in two aspects and seek routes to accelerate IP negotiation definition for projects. First, if industry participants cover all costs, then they should be able to dictate IP terms independent of the physical or digital capabilities used in the course of creating any given invention. On the other hand, if industry participants are only partially covering costs or using lab capabilities on an in-kind basis, then further negotiation on foreground IP ownership and potential royalty fees are anticipated. Easing of regulations to enable more flexibility in responding to the COVID-19 pandemic may foster accelerated innovation in some markets/applications related to managing and fighting the virus.[57] The implications of this deregulation should be considered for extension to other technologies evaluated in the interest of our Nation's competitive advantage.

Recommendation 2.5: *IotF Institute frameworks should leverage economic opportunity zones or similar incentives to attract investment, advance regional development, and catalyze economic growth. (I, G)*

Borrowing from the successful launch of Opportunity Zones in the Tax and Jobs Act of 2017,[58] PCAST recommends that the proposed IotF Institutes leverage the same or similar mechanisms to enable favorable tax treatment in the form of capital gains tax deferrals and/or tax breaks, informed by lessons learned from prior Opportunity Zone investments. PCAST believes similar incentives, together with well-defined IP terms, could be exceptionally valuable in driving collaboration in the advancement of IotF for the economic development of local communities and the Nation as a whole.

The competitive process for participating in an IotF Institute could therefore greatly benefit from the existence of nearby Opportunity Zones, with the decision as to where to locate these being predicated on State and local support. The Institutes' agendas would be driven by industry partners (preferably including multiple large-scale companies), possibly with one or more National Laboratories as well as local colleges or universities, and non-profit organizations. Together, these partnerships would undertake the needed research and development to develop new technology paradigms—including new processes, capabilities, and tools—which would be attractive for regional investment in advanced manufacturing while also supporting the re-establishment of a domestic supply chain.

Recommendation 2.6: *IotF Institute frameworks should be structured to provide both a confluence of leading researchers and a launch pad for early career scientists and engineers. (I, A, G)*

The single greatest resource in the U.S. S&T enterprise is the pool of talented people engaged in R&D. The proposed IotF Institutes should be designed both to leverage existing talent and to nurture the next generation of U.S. scientists and engineers. PCAST envisions the IotF Institutes as a prominent venue for concentrating S&T talent and facilitating the cross-fertilization of ideas among leading researchers from all sectors. PCAST also proposes engaging a diverse set of early career researchers, selected through a highly competitive process, to collaborate with the luminaries of the IotF Institutes. Consequently, this confluence of highly capable, established and early career investigators will provide

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[56] National Academies of Sciences, Engineering, and Medicine. 2020. *A Quadrennial Review of the National Nanotechnology Initiative: Nanoscience, Applications, and Commercialization*. Washington, DC: The National Academies Press. https://doi.org/10.17226/25729

[57] https://www.forbes.com/sites/sallypipes/2020/06/08/covid-19-reveals-the-power-of-deregulation/#405002942147

[58] Tax Cuts and Jobs Act of 2017, Pub. L. No. 115-97, 131 Stat. 2054 (2017)

a new launch pad that helps accelerate the expansion of the next generation of American R&D talent in IotF. Individual IotF Institutes should attain critical mass of talent to address their proposed scope—likely several hundred to a few thousand researchers per Institute. The IotF Institutes should establish a broad range of IotF professional networks and career opportunities to help grow, strengthen, and diversify the U.S. science and engineering workforce. The economic resilience of STEM fields and their corresponding potential to impact economic recovery through innovation and commercialization are also acknowledged.[59]

Recommendation 2.7: *IotF Institutes should facilitate the development of digital twins and help to expand the capabilities of the domestic manufacturing supply chain as a pathway to Factories of the Future. (I, G)*

PCAST envisions *Factories of the Future (FotF)* leveraging advanced physical and virtual assets for dramatically enhanced versatility and efficiency. IotF Institutes will serve as a mechanism for conceiving, testing, and ultimately implementing these benefits. For example, additive manufacturing technologies such as 3D printing will provide on-demand adaptation and customization of parts, enabling on-the-spot repairs and improvements in manufacturing operations. A key enabler for FotF is deployment of digital twins—digital replicas or simulations of all of the factory's assets that allow companies to model, track, and understand their entire factory by mirroring operational performance computationally. Once mature, they enable manufacturing companies to transform operational decision-making and capabilities. Coupling digital twins with additive manufacturing could enable rapid improvements or adjustments to equipment, removing the need to identify a problem, place an order, and wait for parts.

Well-managed factories of today have low failure rates and are essentially operating in a low-number statistics regime. Reliable digital twins, enabled by development and utilization of AI/ML far beyond today's capabilities, would create new opportunities for improvements at scale. Once digital twin status is achieved, the global competitiveness of U.S. manufacturing will be greatly enhanced by facilitating prediction of failure modes well in advance of their physical manifestation and to thereby enable realization of associated competitive improvements in FotF output. The digital twin concept can also be extended beyond the manufacturing plant to encompass entire supply chains: from the supply of raw materials and goods, to individual plants, to downstream distribution of finished goods. These logistics and supply chain relationships are incredibly complex; the combination of reliable digital twins with smart manufacturing (known as Industry 4.0), along with emerging AI/ML (and potentially quantum computing capabilities) could enable competitive benefits for American industry.[60] By bringing together multiple areas of IotF, the IotF Institutes will enable experimentation for both creating new industries and transforming existing ones.

Potential Flagship IotF Institutes

PCAST has several preliminary ideas for IotF Institutes that could catalyze discovery through constructive feedback between fundamental and applied research and product design and development. Such opportunities can spark wholly unanticipated research endeavors and ideas that

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59 See also Section 3 of this report for additional recommendations on Meeting National Needs for STEM Education and a Diverse, Multi-Sector Workforce.

60 National Academies of Sciences, Engineering, and Medicine. 2019. *Strategic Long-Term Participation by DoD in Its Manufacturing USA Institutes: Proceedings of a Workshop*. Washington, DC: The National Academies Press. https://doi.org/10.17226/25440

could lead to world-changing breakthroughs, whether by collocating research endeavors or via remote, virtual interactions. The latter are anticipated and encouraged, especially given the potential of virtual collaborations that has manifested during the current pandemic.

Exemplar IotF Institute on AI and Biotechnology

PCAST's first proposed institute would combine R&D in AI and biotechnology to enhance the Nation's biosecurity, biosafety, and biosphere sustainability. The COVID-19 pandemic has revealed both daunting challenges and important opportunities within the field of biotechnology, particularly at the interface of biology, medicine, and advanced digital technologies. There is a clear need to sustain and expand the Nation's biological and biomedical R&D to improve our ability to manage and treat infectious disease.

This new institute would work to expand analytical methods enabled by AI and ML to advance our understanding of the spread of disease and improve the efficacy of treatments and vaccines—and accelerate their discovery. More fundamentally, an improved understanding of transport phenomena for sub-atomic, atomic, and molecular moieties across the cell membrane and within cells will provide mechanistic foundations for biosecurity, advanced therapies, and food security for the Nation. This institute is a strong candidate for piloting the Accelerated Discovery Workflow described in Section 1 of this report.

More broadly, the U.S. bioeconomy—including the "infrastructure, innovation, products, technology, and data derived from biologically-related processes and science"[61]—has been estimated to comprise roughly 5% of the American gross domestic product, amounting to over $950 billion.[62] This vast sector spans our food supply and health care systems, myriad commercial products that affect all aspects of our daily lives, and fundamental and applied research that explore the very building blocks of life. Indeed, the precise physical and chemical processes that govern the structure and function of cell biology have not yet been fully elucidated.

As part of *Foundries for American Biotechnology*[63] (FAB), current efforts are underway to establish a set of capabilities involving the DoD, the Department of Health and Human Services (HHS), DOE, and NIST in the form of a *National Biodesign Institute* (NBI), a *National Biotechnology Accelerator* (NBiotA), and a *Biotechnology Institute of Manufacturing Excellence* (BIOME). DOE's recently launched National Virtual Biotechnology Laboratory (NVBL), a consortium of DOE National Laboratories,[64] is primarily focused on testing capabilities, therapeutics, epidemiological and logistical support, and supply chain.

The IotF Institute on AI and Biotechnology could stimulate a longer term, large-scale (100–3000 researchers) initiative to achieve sustainable biotechnology solutions, maintain national security, cultivate advanced biological R&D enabled by HPC, develop advanced tools for precision gene editing and design-oriented biological engineering, support the scalable realization of synthetic biology, and address the needs of the growing and multi-faceted bioeconomy. Although achievement of the necessary scale and critical mass for this far-reaching endeavor places it among our long-term

61 https://www.whitehouse.gov/wp-content/uploads/2019/10/Summary-of-White-House-Summit-on-Americas-Bioeconomy-October-2019.pdf

62 National Academies of Sciences, Engineering, and Medicine. 2020. *Safeguarding the Bioeconomy.* Washington, DC: The National Academies Press. https://doi.org/10.17226/25525

63 "HHS Pioneers First Foundry for American Biotechnology," https://www.hhs.gov/about/news/2020/02/10/hhs-pioneers-first-foundry-for-american-biotechnology.html, accessed May 22, 2020.

64 "National Virtual Biotechnology Laboratory (NVBL)." https://science.osti.gov/nvbl. Accessed June 22, 2020.

objectives, the pressing public health challenges of COVID-19 underscore a need to begin immediately. The Nation should not wait for another global health crisis to undertake the measures necessary to secure public health or any of the other tremendous benefits that this institute will enable.

Exemplar IotF Institute on Generative Design in Advanced Manufacturing

The second proposed Institute focuses on the R&D required to advance AI and ML tools and capabilities relevant to generative design in advanced manufacturing. Given the clear and far-reaching implications of AI and ML that continue to emerge in nearly all areas of S&T, another institute would ideally focus on R&D for leveraging the myriad data-intensive benefits of AI and ML within the particular context of advanced manufacturing and generative design, while also addressing a pressing need to expand U.S. manufacturing capabilities in the context of advanced communication integration & infrastructure (5G and beyond).

This flagship IotF Institute on Generative Design in Advanced Manufacturing would complement and augment the Manufacturing USA institutes (including *America Makes* for additive manufacturing, the *Advanced Robotics for Manufacturing Institute*, and advanced materials institutes including *Lightweight Innovations for Tomorrow*, the *Institute for Advanced Composites Manufacturing*, and the *Advanced Functional Fabrics of America Institute*), as well as leveraging and extending current investments and established programs at National Laboratories for capabilities such as additive and generative design.[65]

The new Institute could build off other investments in AI/ML through a portfolio spanning R&D in generative design, prediction of optimal methods for packing and managing parts, and tracking and assessment of supply chains. As quantum computers advance, they could potentially be used to amplify the power of AI/ML in this context within an Accelerated Discovery Workflow. In addition to being a fundamental enabler of U.S. competitiveness in advanced communications, the sensing and connectivity that is being facilitated by 5G+ networks would provide a rich source of highly granular data that may yield new AI/ML-driven benefits for America's manufacturing enterprise.

Administration of IotF Institutes: Addressing Hurdles in Efficacy & Efficiency in the Laboratory Enterprise

PCAST proposes that the IotF Institutes be administered by DOE. The U.S. National Laboratories operated by the DOE have been a cornerstone of the R&D ecosystem over the past several decades, enabling pivotal advancements in nuclear energy, HPC, biology, and numerous other key areas of technology. Historically, the labs were chartered with the capability to attack huge problems for the benefit of the Nation, and to conduct high-risk/high-cost research that is generally not feasible for private industry or academia.

However, in recent years, the Laboratories have faced significant operational challenges, due in part to increasingly granular budgetary control, ultimately resulting in the phenomenon of "budget atomization," whereby ever-smaller increments of funding are allocated to individual projects. Consequently, many researchers are forced to pursue a piecemeal approach to research that involves multiple small proposals and correspondingly greater reporting requirements, subsequently leading to less time for actual research and thus an overall reduction in value for the R&D enterprise. Moreover,

[65] For example, Sandia National Laboratory's PLATO tool, a digital environment for topology optimization-based design. https://www.sandia.gov/plato3d/index.html

this arrangement likely incentivizes risk aversion, during a time in which rapidly increasing global competition actually indicates a greater need for bold approaches to innovation.

Multiple previous examinations of the Laboratories' operation and performance have noted this problematic trend. Most recently, the 2015 final report of the Commission to Review the Effectiveness of the National Energy Laboratories (CRENEL) likewise surveyed past reports, specifically noting that substantive action had yet to be taken in response to many previous recommendations for operational improvements. The CRENEL report notes that a Laboratory's "budget flexibility depends on both the legal restrictions imposed by Congress in their allocation of funding and the granularity of management by each DOE program office."[66] The atomization problem, which also includes the impact of long and cumbersome congressional approvals necessary to permit the movement of funds above a statutorily defined ceiling between certain projects, is a rather complex issue and varies across the program offices and laboratories. PCAST ultimately views these as well intended, yet often inadequately functioning attempts at quality control.

Another important observation is that while the statutorily granted transactional authorities for DOE Laboratories are rather similar to those provided to the National Aeronautics and Space Administration and DoD, their application is different. Consequently, PCAST suggests seeking harmonization according to the <u>least restrictive</u> of the current funding authorization processes deployed across these agencies, and applying them to the IotF Institutes so that overall efficiency and impact of the associated IotF Institutes are maximized.

Finally, compensation, hiring, and retention of talent within the IotF Institutes will require careful consideration. The different elements of our Nation's S&T enterprise embrace distinct compensation models that are inevitably revealed in cross-sector and multi-enterprise collaborative efforts (Section 1). Although pay is only one facet of a researcher's work experience, progressive compensation strategies should be proactively developed and deployed by IotF Institute administrators to assure continued talent balance across the participating organizations in our Nation's S&T enterprise.

[66] DOE. 2015. *Securing America's Future: Realizing the Potential of the Department of Energy's National Laboratories.* Final Report of the Commission to Review the Effectiveness of the National Energy Laboratories.

3. Meeting National Needs for a Diverse, Multi-Sector IotF Workforce

In an increasingly competitive global S&T arena, ensuring that the American workforce is prepared for the future is critical to retaining U.S. economic and S&T leadership. Furthermore, the massive economic disruption and loss of jobs caused by the COVID-19 pandemic has brought into stark relief the challenges faced by many workers. PCAST sees an urgent need to improve access to high quality education and training programs in STEM in order to build the Nation's STEM capacity and lay the foundation for the Workforce of the Future.

For the Nation to succeed in the Second Bold Era of Science and Technology, we must leverage the full potential of our human resources, which will require a commitment to ensuring inclusion of individuals who have been underserved and underrepresented in STEM—whether on the basis of race, ethnicity, gender, sexual orientation, disability, socioeconomic background, or geographic location. Broadening access to those who are in underrepresented and underserved communities—including those who have been displaced by pandemic-related economic disruption—can unleash new potential and create pathways to economic prosperity while helping to meet critical workforce needs in STEM. Empowering individuals to improve their skills throughout their lifetime will help elevate America's IotF workforce to its greatest potential. Achieving these goals will require nothing short of significant and sustained actions across all sectors, especially the public sector (Federal, State, and local government) and the private sector (corporations and professional associations).

PCAST has identified two priorities where actions by both the U.S. Government (G) and industry (I) partners, in coordination with academia (A), are needed.[67]

***PRIORITY 1*: Build the Workforce of the Future by creating STEM training and education opportunities for individuals from all backgrounds, including underrepresented and diverse populations and individuals from non-STEM backgrounds.**

***PRIORITY 2*: Create new curricula and universal skills-based licenses and certifications for IotF.**

The specific recommendations associated with each priority provide guidance for actions that can and should be taken by various sectors to advance the U.S. STEM Workforce of the Future, including the Federal Government. These priorities for workforce development and training are intended to complement the priorities and recommendations offered in other sections of this report, as well as ongoing Administration initiatives such as the *National Strategy for STEM Education*.[68]

Priority 1: Build the Workforce of the Future by creating STEM training and education opportunities for individuals from all backgrounds, including underrepresented, underserved, and diverse populations and individuals from non-STEM backgrounds.

Recommendation 3.1: ***Employers, academic institutions, professional societies, and other partners should develop programs to provide non-STEM workers with professional competencies that will grant them a role in the Workforce of the Future.*** Public- and private-sector employers should be recruited to pledge support for the hiring of newly skilled STEM workers, especially those from non-traditional backgrounds, into IotF and other STEM and skilled technical workforce positions. (I, G, A)

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[67] See also the recommendations in Section 1 related to workforce development for American Global Leadership in Industries of the Future.

[68] https://www.whitehouse.gov/wp-content/uploads/2018/12/STEM-Education-Strategic-Plan-2018.pdf

Recommendation 3.2: ***NSF should establish a grant program to create and pilot multi-sector, Workforce of the Future, STEM Retraining Boards*** that connect individuals to new or existing opportunities for continuing education, training, certification, and reskilling in IotF and STEM fields. (G)

Within the NSF Directorate for Education and Human Resources, a new program should be established to oversee and provide 50 initial competitive grants of up to $1,000,000 each for the formation of local or regional U.S. STEM Retraining Boards by 2022. The purpose of these Boards is to connect workers with education and training opportunities that will empower them to participate in IotF, either as scientists and engineers or as members of the Nation's skilled technical workforce.[69]

Boards could be structured as public-private partnerships among local governments, regional universities, community colleges, industry certification institutions, local employers, and trade groups. By 2025, the Boards collectively should aim to bring millions of Americans from non-technical backgrounds into IotF and other STEM jobs, and to strengthen the STEM and technical skills of workers across all occupational fields. Participation in the proposed STEM retraining boards is a concrete opportunity for companies, trade groups, and other potential partners to help realize the Pledge to America's Workers[70] (to expand programs that educate, train, and reskill American workers from high school age to near-retirement) in STEM fields.

Increasing diversity in the workplace is known to improve effectiveness by bringing a wider array of perspectives, skills, and talents to solving problems. Furthermore, opportunities to incorporate non-technical skills into STEM training may make STEM opportunities more appealing to a broader range of individuals, while enriching the skill sets and capabilities of all STEM workers. In building the Workforce of the Future, a diverse talent pool will support responsible development and use of emerging technologies like AI, QIS, biotechnology, and advanced manufacturing. This effort should draw upon the largest pool of talent possible, which will require a commitment to ensuring that populations historically underrepresented and underserved in S&T, on account of race, ethnicity, gender, economic class, geographic location, disability, or sexual orientation have the ability to take on opportunities in the emerging IotF. Ensuring that opportunities in the Workforce of the Future are open to all Americans will require data to establish current patterns, to identify emerging trends, and to recognize best practices in training, retraining, and continuing education.

Priority 2: Create new curricula and universal skills-based licenses and certifications for IotF.

Recommendation 3.3: ***Commit Federal funds, matched by support from the private sector and universities—including endowments, foundations, or in-kind support—to create industry-recognized curricula and work-based learning and training programs in the IotF areas of QIS, AI, and advanced manufacturing through public–private partnerships. (I, A, G)***

Recommendation 3.4: ***These public-private partnerships should also create universal skills-based licenses and certifications targeting IotF, and employers should commit to using skills-based[71] certifications as the basis for training/education and job descriptions using informed recommendations from representatives from industry and professional societies.*** PCAST

[69] Defined as "workers who use science and engineering skills in their jobs but do not have a bachelor's degree" by a recent National Science Board Task Force, https://www.nsf.gov/nsb/publications/2019/nsb201923.pdf

[70] https://www.whitehouse.gov/presidential-actions/executive-order-establishing-presidents-national-council-american-worker/; https://www.whitehouse.gov/pledge-to-americas-workers/

[71] https://www.whitehouse.gov/presidential-actions/executive-order-modernizing-reforming-assessment-hiring-federal-job-candidates/

recommends a high sense of urgency in establishing these certifications, and industry partners would be well positioned to pledge to aim for 50% of hires into suitable technology-based positions from the pool of newly licensed/certified individuals by 2025. (I, A, G)

Overly specialized, non-standard job specifications make it difficult for potential hires, particularly those from nontraditional backgrounds, to apply for STEM jobs and for employers to fill positions. Establishing industry-recognized credentials and standards would benefit both the recruitment and retention of individuals into STEM at all stages of the STEM pipeline.

As noted in Sections 1 and 2, one of the major challenges to building critical capacity in QIS and AI is that U.S. colleges and universities as a whole do not have common, recognized curricula in place to train the next generation of specialists in these fields. Public-private partnerships should be established to support institutions of higher education across the United States to create novel curricula and training programs to spark undergraduates, graduate students, post-doctoral fellows, educators, and faculty to train in quantum computing and AI. Opportunities for U.S. students to learn via study and practice abroad also could be included.

Educational programs designed with industry-recognized, skills-based credentials would give students confidence their degrees are preparing them to succeed in the jobs of tomorrow. For individuals already in the workforce, certifications would provide guidance for reskilling, upskilling, and making informed career advancement decisions resulting in increased economic prosperity. Such credentialing programs could be informed by existing models such as certification for public accountants (CPAs), licensed nurse practitioners (LNPs), and paralegals (CPs). Such programs could also consider a continuing education model for updating workers' skills as these fields continue to advance, as is done, for example, in medical professions through continuing medical education.

In light of the need to adapt academic programs to the constraints posed by COVID-19, PCAST recommends a concerted focus on training courses based upon both in-person and virtual learning for the near term. In addition, partnership-driven opportunities for experiential learning through research, internships, and apprenticeships will help build the necessary skills to meet the growing demands of the future STEM workforce at all education and training levels. These can also reinforce positive relationships between local public and land-grant universities, which drive regional innovation and economic development of the States. Certification and training programs that offer flexibility and affordability to students and workers should be strengthened through partnerships centered around a university's mission, while complementing efforts at the State and local level. These should focus on including historically underserved or underrepresented populations.

For employers, committing to create skills-based, standard job codes tied to industry certifications will clarify hiring requirements for firms seeking to fill positions and provide a clear understanding of what prospective employees are capable of doing. Funding for these IotF curricula and training programs would come from a variety of sources. Government support should come from NSF and other Federal agencies, through at least FY 2025. These public monies would be matched by funds from private-sector partners, university endowments or in-kind support, and State funds where possible.