



EXECUTIVE SUMMARY OF THE REPORT TO THE PRESIDENT

Supercharging Research: Harnessing Artificial Intelligence to Meet Global Challenges

Executive Office of the President
President's Council of Advisors on
Science and Technology

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EXECUTIVE OFFICE OF THE PRESIDENT
PRESIDENT'S COUNCIL OF ADVISORS ON SCIENCE AND TECHNOLOGY
WASHINGTON, D.C. 20502

President Joseph R. Biden, Jr.
The White House
Washington, D.C.

Dear Mr. President,

Your President's Council of Advisors on Science and Technology (PCAST) is excited by the forward-looking approach that your Administration has taken to advance the safe and effective use of artificial intelligence (AI).^{1,2,3} As requested in your landmark [Executive Order on the Safe, Secure, and Trustworthy Development and Use of Artificial Intelligence](#), we are pleased to report here on the *possibilities* that AI can enable when applied to research to address major societal and global challenges.

AI will fundamentally transform the way we do science. Researchers in many fields are already employing AI to identify new solutions to a wide array of long-standing problems. Today, scientists and engineers are using AI to envision, predictively design, and create novel materials and therapeutic drugs. In the near future, AI will enable unprecedented advances in the social sciences, both through new methods of analyzing existing data and the development and analysis of new kinds of anonymized and validated data. Such advances will allow government to better understand how policies affect the American people, and improve those policies to better meet societal needs and challenges. AI will also allow researchers to run millions of computer-based simulated experiments quickly to provide guidance about the most important real-world experiments to run. In industrial laboratories, rich simulations will be able to identify hazards or faults in design so that scientists and engineers can create safer, scalable, and efficient products that American industry and American consumers can depend on. In sum, AI is revolutionizing the research process, enriching scientific models, and accelerating data generation and analysis, with impacts that will be far-ranging.

In addition to its opportunities, we must recognize that AI can create new issues and challenges, such as distilling errors and biases embedded in skewed training data, the enormous—and increasing—amounts of energy required for the computational processes, the possibility that faulty science could be unwittingly generated, and the ease with which nefarious actors could use new powerful AI technologies for malicious purposes. . Expert human supervision, building protections into the AI algorithms, and a culture of responsible use that includes appropriate application of regulatory frameworks, as outlined in your [Blueprint for an AI Bill of Rights](#) and the [AI Risk Management Framework](#) from the National Institute of Standards and Technology, will be essential to mitigating the weaknesses and dangers of AI. Fortunately, reproducibility and validation are core tenets of the

¹ The White House. (2022 October). [Blueprint for an AI Bill of Rights: Making Automated Systems Work for The American People](#).

² Executive Order 14110, 88 FR 75191. (2023 October). "[Safe, Secure, and Trustworthy Development and Use of Artificial Intelligence](#)."

³ The White House Office of Management and Budget. (2024 March). [Advancing Governance, Innovation, and Risk Management for Agency Use of Artificial Intelligence](#). [Memo M-24-10]

scientific method. As such, the scientific community is already engaged in vibrant and pathbreaking research on AI reproducibility, testing, and evaluation so that researchers—and everyone—will eventually be able to use AI tools with the same confidence with which we use calculators.

Ultimately, our vision is that the responsible use of AI will empower scientists and engineers to leverage the opportunities of this transformative technology while navigating and mitigating its weaknesses.

Ultimately, our vision is that the responsible use of AI will empower human researchers to leverage the opportunities of this transformative technology while navigating and mitigating its weaknesses.

Per your Executive Order, and building on the bold work of your Administration, PCAST offers findings and recommendations for action that will help the United States to harness the full potential of AI to equitably and responsibly supercharge research to meet the world's challenges.

Sincerely,

The President's Council of Advisors on Science and Technology

Executive Summary

Artificial Intelligence (AI) has the potential to revolutionize our ability to address humanity’s most urgent challenges by providing researchers with tools that will accelerate scientific discoveries and technological advances. Generative AI, which can create content based on vast data sets and extensive computation, is poised to be particularly transformative. Examples of generative AI include large language models, image generating models, and generative scientific models. In his comprehensive [Executive Order on the Safe, Secure, and Trustworthy Development and Use of Artificial Intelligence](#), issued on October 30, 2023, President Biden charged PCAST to report on “the potential role of AI...in research aimed at tackling major societal and global challenges.” PCAST is pleased to offer this report in fulfillment of this charge.

With well-designed, equitably shared, and responsibly used infrastructure, AI will enable scientists to address urgent challenges, including improving human health and enhancing weather prediction in a time of climate change. AI can help explore long-standing scientific mysteries that inspire and stretch human creativity, such as uncovering the origin and evolution of the universe. AI will also help researchers address continuing national needs, from accelerated semiconductor chip design to the discovery of new materials to address our energy needs. Furthermore, AI is starting to remove barriers that make scientific research slow and expensive, for instance by providing the means for rapidly identifying the best drug candidates for testing (thus reducing the number of expensive laboratory trials), helping to optimize experimental designs, and uncovering connections in data much more efficiently than can be done by hand or using traditional data science methods. If basic AI resources, validated data, and scientific tools and training are made broadly accessible, AI technologies have the potential to democratize scientific knowledge,⁴ bringing interconnected technical concepts to many more people and enabling diverse researchers to bring their expertise and perspectives to societal and global challenges.

Just as with any other new tool or technology, realizing the potentials of AI will require addressing its limitations. These issues include misleading or incorrect results, perpetuation of bias or inequity⁵ and sampling errors from patterns embedded in the model-training data, limited access to high quality training data, the challenges of protecting intellectual property and privacy, the significant energy required to train or deploy a model or run the AI algorithms, and the risk that bad or nefarious actors will use readily available AI tools for malicious purposes. Many public and private sector activities addressing these issues are already underway, including government efforts tasked under the October 2023 Executive Order on AI. Reproducibility and validation are key principles underlying scientific integrity and the scientific method and must continue to be held at high value as we develop a culture of responsible AI use and expert human supervision of AI applications.

AI has the potential to transform every scientific discipline and many aspects of the way we conduct science. Scientists are already employing AI to create new functional materials that we presently do not know how to design; these include superconductors and thermoelectric materials which would not only enhance our energy efficiency but also reduce our carbon footprint. In a similar vein, AI models are helping researchers create new designs for manufacturing processes and products, and

⁴ Dessimoz, C. and Thomas, P. (2024 March). [AI and the democratization of knowledge](#). *Scientific Data*.

⁵ Birhane, A. (2022 October). [The unseen Black faces of AI algorithms](#). *Nature*.

develop new drug therapies which in the future could enable individualized treatment of specific cancers and viruses. AI models are also helping engineers design semiconductor chips, producing better designs with less human effort and time. In health care, AI technologies are creating new ways to analyze a broad spectrum of medical data for applications like the early diagnosis of diseases⁶ that can lead to timely intervention and the detection of medical errors.⁷ PCAST also foresees widely available AI-powered ultra-personalized medicine tailored to a specific individual and disease process that will include details of medical history, genetic information, and signals, such as how healthy and unhealthy cells are behaving.

AI is also transforming science by improving our scientific models. In climate science, AI models are starting to enhance weather prediction, as well as advancing whole-earth models for water management, greenhouse gas monitoring, and predicting the impacts of catastrophes. Scientists have already used AI to successfully predict the structure of proteins; new foundation models will unlock more secrets of cellular biology and power computer simulations of intracellular interactions that can be used to explore new therapies. AI models promise to help us understand the origin of our universe by allowing us to test numerous cosmological hypotheses via rapid simulations. Such AI-enabled modeling may even help scientists discover new laws of physics.

AI will enable unprecedented advances in the social sciences, complementing qualitative methods with new quantitative techniques for analyzing existing data, as well as the development and analysis of newer types of data, e.g., step counts on smartphones, anonymized data drawn with permission from search and browsing, or images posted on social media. AI could supercharge research using vast data sets, such as those that have long been collected and curated by federal statistical agencies—ideally complemented by those held by the private sector—as input for designing effective federal policies. Application of AI to these long-standing and newer social science data sets could facilitate more effective, responsive, and fairer data-driven policymaking and delivery of services.

These few examples of AI-assisted research illustrate that with the responsible use of AI technology, human scientists will be empowered to realize transformational discoveries. Furthermore, PCAST expects that responsible sharing of basic AI resources will help to democratize science and tackle major societal and global challenges.

The use of AI for science and technology research is accelerating rapidly across the globe and therefore demands our commitment to U.S. leadership in the applications of this powerful new tool. Building on the work of the Biden Administration, the United States must act boldly and thoughtfully to maintain our nation’s lead in research, in the innovative applications of AI, and in establishing frameworks and norms for the safe and responsible use of AI. In this report, PCAST offers five specific findings and recommendations for action that will help the U.S. to harness the full potential of AI to equitably and responsibly supercharge scientific discovery.

⁶ Bera, K. et al. (2019 August). [Artificial intelligence in digital pathology - new tools for diagnosis and precision oncology](#). *Nature Reviews Clinical Oncology*.

⁷ Nguyen, V. et al. (2023 November). [Efficient automated error detection in medical data using deep-learning and label-clustering](#). *Scientific Reports*.

Summary of Recommendations

Recommendation 1: Expand existing efforts to broadly and equitably share fundamental AI resources.

Extensive support for widely accessible shared models, data sets, benchmarks, and computational resources is essential to ensuring that academic researchers, national and federal laboratories, and smaller companies and non-profit organizations can use AI to create benefits for the nation. In the U.S., the most promising effort in this direction is the National Artificial Intelligence Research Resource (NAIRR), which is currently a pilot project. PCAST recommends that the NAIRR pilot be expeditiously expanded to the scale envisioned by the NAIRR Task Force⁸ and fully funded. The full-scale NAIRR, together with industry partnerships and other AI infrastructure efforts at both the federal and state levels, could serve as a stepping stone towards AI infrastructure projects at the national or international level to facilitate high-impact research.

Recommendation 2: Expand secure access to federal data sets for approved critical research needs, with appropriate protections and safeguards.

The benefits of allowing limited, secure access to federal data sets by approved researchers, as well as allowing the release of carefully anonymized versions of such data sets to curated resource centers such as NAIRR, are immense. PCAST strongly encourages expansion of existing pilot programs for secure data access and the development of guidelines for federal database management that incorporate cutting-edge privacy protection technologies as they become available. There is great potential to use modern AI technologies to automate aspects of the curation of such data sets. PCAST encourages the use of AI to improve data curation as a long-term goal of federal data sharing initiatives such as data.gov.

PCAST endorses the efforts of federal agencies to mandate responsible sharing of data sets arising from the research that they fund or conduct.⁹ We encourage further enforcement of such mandates, to include sharing of AI models trained on data from federally funded research, in conjunction with sufficient resources to support the required actions.

Recommendation 3: Support both basic and applied research in AI that involves collaborations across academia, industry, national and federal laboratories, and federal agencies as outlined in the vision for the NAIRR developed by the NAIRR Task Force.

The boundaries between federally funded academic research and private sector research are hazy. Many researchers move among affiliations with academic institutions, non-profit organizations, and/or private companies, and a significant share of all AI research and development (R&D) is

⁸ National Artificial Intelligence Research Resource Task Force. (2023 January). [Strengthening and Democratizing the U.S. Artificial Intelligence Innovation Ecosystem: An Implementation Plan for a National Artificial Intelligence Research Resource](#).

⁹ The White House Office of Science and Technology Policy. (2022 August). [Ensuring Free, Immediate, and Equitable Access to Federally Funded Research](#).

currently supported by private companies.¹⁰ To capitalize fully on the potential benefits of AI for science, research that involves a breadth of promising and productive hypotheses and approaches must be supported. This may require that funding agencies broaden their postures regarding how to work with industry and which researchers can be supported in order to facilitate innovative research efforts and collaborations among different sectors. Examples of such collaboration could include creation of high quality curated public scientific data sets from multiple sources or the creation of multimodal foundation models.¹¹

Recommendation 4: Adopt principles of responsible, transparent, and trustworthy AI use throughout all stages of the scientific research process.

Managing the risks of inaccurate, biased, harmful, or non-replicable findings from scientific uses of AI should be planned from the initial stages of a research project rather than performed as an afterthought. PCAST recommends that federal funding agencies consider updating their responsible conduct of research guidelines to require plans for responsible AI use from researchers. These plans should include recommended best practices from agency offices and committees that address potential AI-related risks and describe the supervision procedures for use of any automated process.¹² To minimize additional administrative burden on researchers and build a culture of responsibility, after enumerating major risks, agencies should provide model processes for risk mitigation.

Parallel to this, agencies such as the National Science Foundation (NSF) and the National Institute of Standards and Technology (NIST) should continue supporting research in the scientific foundations of responsible and trustworthy AI. This research should include the development of standard benchmarks to measure AI model properties such as accuracy, reproducibility, fairness, resilience, and explainable AI, as well as AI algorithms that monitor themselves for these properties and adjust when the benchmarks are not within defined norms. Another goal of such research should be the development of tools to evaluate biases in data sets and to distinguish synthetic data from real world data.

Recommendation 5: Encourage innovative approaches to integrating AI assistance into scientific workflows.

The scientific enterprise is an excellent "sandbox" in which to practice, study, and assess new paradigms of collaboration between humans and AI assistants. The objective should not be to maximize the amount of automation, but to allow human researchers to achieve high quality science that utilizes AI assistance responsibly.

Funding agencies should recognize the emergence of these new workflows and design flexible procedures, metrics, funding models, and challenge problems that encourage strategic

¹⁰ National Science Foundation. (Accessed 23 April 2024). [The State of U.S. Science and Engineering 2022 \(Figure 16\)](#).

¹¹ A *foundation model* is an ML model trained (often at great computational expense) on a broad range of data, which can then be fine-tuned relatively cheaply for more specialized applications. For more discussion, see Bommasani, R. et al. (2022 July). [On the Opportunities and Risks of Foundation Models](#). arXiv.

¹² National Institute of Standards and Technology. (2023 November). [Artificial Intelligence Safety Institute Consortium](#). Federal Register.

experimentation with new AI-assisted ways to organize and execute a scientific project. Implementation of these workflows also present opportunities for researchers from a variety of disciplines, such as human factors and industrial and organizational psychology, to advance our knowledge in the area of human-machine teaming.

More broadly, incentive structures across funding agencies, academia, and the academic publishing industry may need to be updated to support a broader range of scientific contributions, such as curating a high quality and broadly usable data set that might not be given sufficient recognition by traditional metrics of research productivity.

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