Brookhaven National Laboratory

U.S. Department of ENERGY

FASST & Related AI Initiatives

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@BrookhavenLab

Global Techno-Economic Landscape

1. AI is rapidly becoming the **dominate driver/signal of techno-economic progress and competition in the next decade.**
2. **AI is pervasive and is becoming ubiquitous** across dozens of economically critical domains.
3. Massive competition/positioning in AI will exist **between western democracies, semi-aligned states, and adversaries.**
4. AI provides state and non-state actors with the **potential for nonlinear progress in technological, economic, and national security domains.**
5. Exploiting advantages through strategic investments in non-commercial AI capabilities rather than on **mitigating AI risks.**
6. Private sector is making exponentially fast progress on Generative AI.

2022 Workshops Recognized this Trend: AI4SES Six Conceptual Clusters

AI for advanced properties inference and inverse design

Energy Storage
Proteins, Polymers,
Stockpile modernization

AI and robotics for autonomous discovery

Materials, Chemistry, Biology
Light-Sources, Neutrons

AI-based surrogates for high-performance computing

Climate Ensembles
Exascale apps with surrogates
1000x faster => Zettascale now

AI for software engineering and programming

Code Translation, Optimization
Quantum Compilation, QAlgs

AI for prediction and control of complex engineered systems

Accelerators, Buildings, Cities
Reactors, Power Grid, Networks

Foundation models for scientific knowledge tasks

Hypothesis Formation, Math
Theory and Modeling Synthesis,

Source: https://www.anl.gov/ai-for-science-report

White House Executive Order on AI (October 30, 2023)

AI for Science, Energy, and National Security. Consistent with DOE's priorities in the May 2023 AI for Science, Energy, and Security report, DOE is tasked with expanding **partnerships with industry, academia, other agencies, and international partners** to utilize DOE's computing capabilities and AI testbeds to **build foundation models that support new applications in science, energy, and national security**, including community preparedness for climate-related risks, enable clean-energy deployment (including addressing delays in permitting reviews), and enhance grid reliability and resilience

DOE is also charged with issuing a public report "enable the provision of clean, affordable, reliable, resilient, and secure electric power to all describing the potential for AI to improve planning, permitting, investment, and operations for electric grid infrastructure and to Americans." DOE is also tasked as the lead agency, through the National Nuclear Security Administration, to **reduce the risks at the intersection of AI and chemical, biological, radiological, and nuclear (CBRN) threats**. DOE is required to develop testbeds and "tools to evaluate AI capabilities to generate outputs that may represent nuclear, nonproliferation, biological, chemical, critical infrastructure, and energy-security threats or hazards" and "develop model guardrails that reduce such risks."

DOE Office of Critical and Emerging Technologies Announces FASST

Frontiers in Artificial Intelligence for Science, Security and Technology (FASST)

The proposed **Frontiers in AI for Science, Security, and Technology (FASST)** initiative leverages DOE's enabling infrastructure to deliver key assets for the national interest:

- **Advance National Security**. The development of AI models for national security applications, such as threat detection and strategic deterrence is crucial to maintaining America's defensive posture.
- **Attract and build a talented workforce**. FASST is the most ambitious AI initiative of its kind. This mission will attract, train, and retain top scientific talent for a leading capability deployed in the public interest.
- **Harness AI for Scientific Discovery**. FASST will develop AI tools that will dramatically reduce the time to discovery and extend the nation's competitive edge in technological innovation.
- **Address Energy Challenges**. FASST will unlock new clean energy sources, optimize energy production, and improve grid resilience, and build tomorrow's advanced energy economy. America needs low-cost energy to support economic growth and FASST can help us meet this challenge.
- **Develop technical expertise necessary for AI governance**. FASST will provide insight and independent expertise to quickly inform and validate standards and regulations for a responsible and safe AI industry.

The Department of Energy AI Act:

Authorizes the Frontiers in Artificial Intelligence for Science, Security, and Technology (FASST) initiative at DOE. Establishes a network of AI research clusters built on DOE's existing ecosystem of computing capabilities and research facilities at National Labs. 6 days ago

JULY 10, 2024

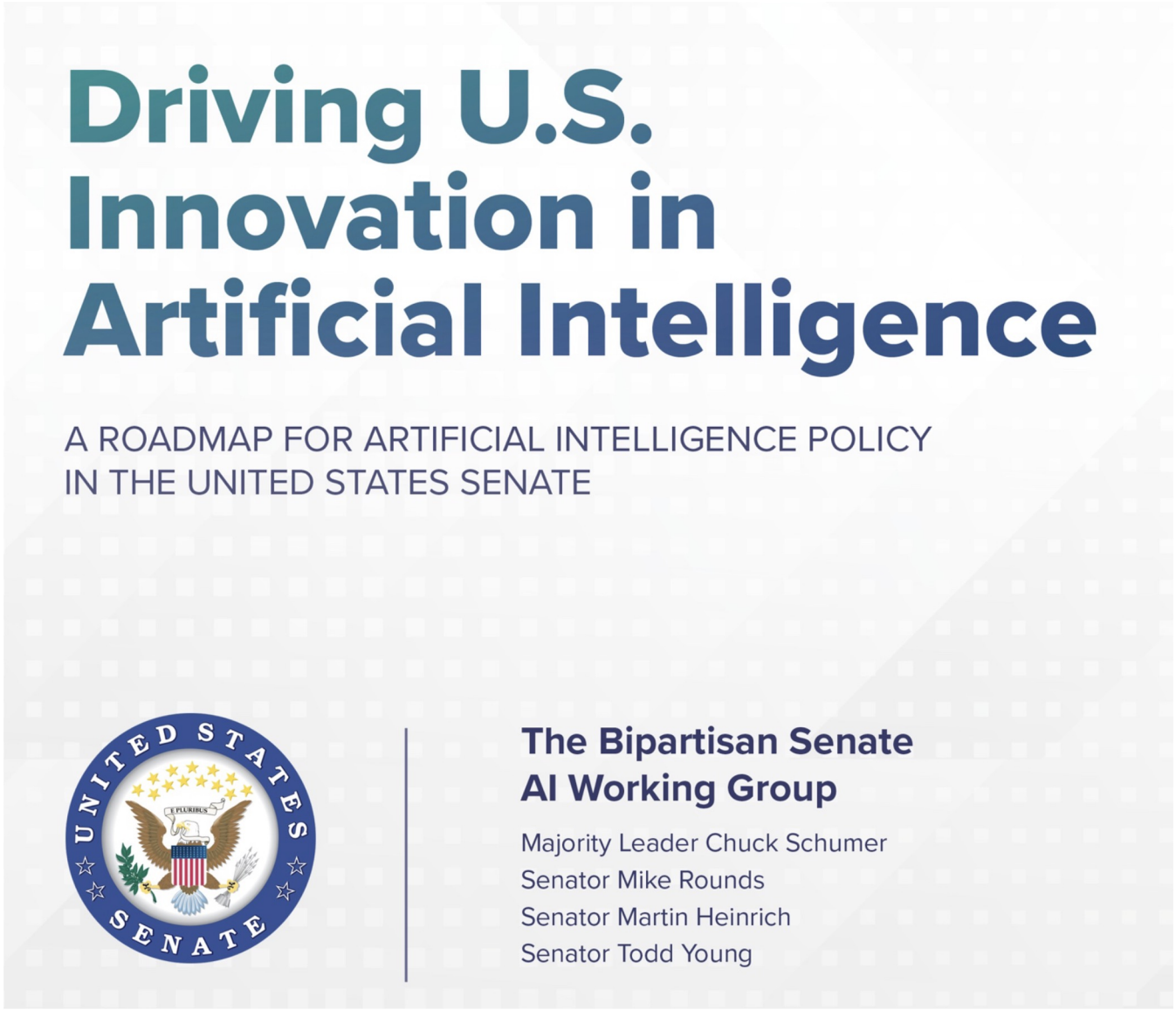
MANCHIN, MURKOWSKI INTRODUCE BIPARTISAN LEGISLATION TO ADVANCE DEPARTMENT OF ENERGY AI RESEARCH FOR SCIENCE, SECURITY, AND TECHNOLOGY

Washington, DC — Today, U.S. Senator Joe Manchin (I-WV), Chairman of the U.S. Senate Energy and Natural Resources Committee, and Senator Lisa Murkowski (R-AK) introduced the bipartisan *Department of Energy AI Act* to advance American leadership in artificial intelligence (AI) by harnessing the existing National Laboratory infrastructure and workforce at the Department of Energy (DOE).

"As AI technology takes the world by storm, the United States needs to meet the moment quickly and effectively before our adversaries do. The DOE and its network of National Laboratories are ready and able to bring our nation to the next level of scientific discovery and global competitiveness through the innovation of safe and responsible AI," **said Chairman Manchin.** "This bipartisan legislation will leverage the agency's existing world-class laboratory test facilities, scientific workforce, and advanced computing resources to strengthen our country's AI capabilities to remain the superpower of the world in energy, national security, and economic competitiveness. Deploying our existing lab infrastructure and scientific expertise for AI instead of starting from scratch will also safeguard taxpayer dollars and allow for us to move quickly. As Chairman of the Senate Energy and Natural Resources Committee, I am proud to work with my friend, Senator Murkowski, on this crucial legislation and I encourage my colleagues on both sides of the aisle to support this initiative to further unlock the groundbreaking potential of AI."

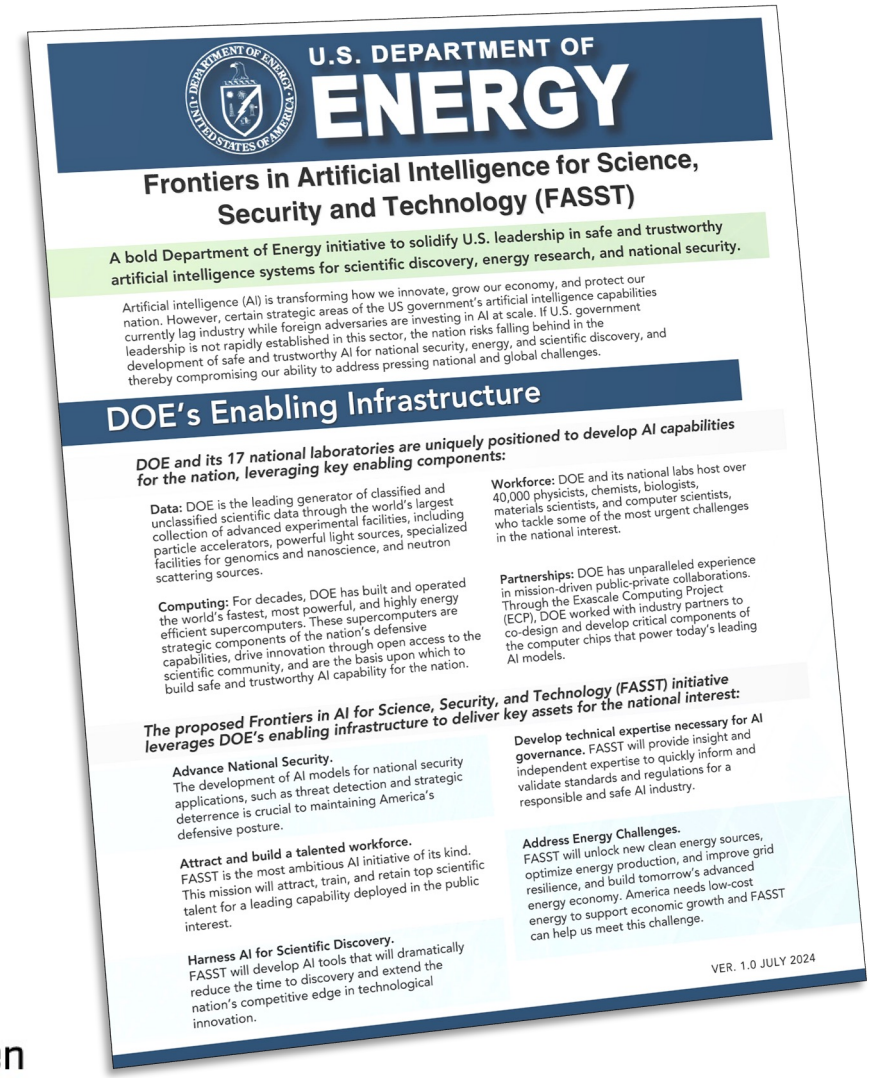
Majority Leader Schumer and Co. Ask for $32B/yr for Non-defense AI Research and Development

$32B/yr for non-defense agency AI



May 14-SENATE ROADMAP

DOE FASST Overview



U.S. DEPARTMENT OF ENERGY

Frontiers in Artificial Intelligence for Science, Security and Technology (FASST)

A bold Department of Energy initiative to solidify U.S. leadership in safe and trustworthy artificial intelligence systems for scientific discovery, energy research, and national security.

Artificial intelligence (AI) is transforming how we innovate, grow our economy, and protect our nation. However, certain strategic areas of the US government's artificial intelligence capabilities currently lag industry while foreign adversaries are investing in AI at scale. If U.S. government leadership is not rapidly established in this sector, the nation risks falling behind in the development of safe and trustworthy AI for national security, energy, and scientific discovery, and thereby compromising our ability to address pressing national and global challenges.

DOE's Enabling Infrastructure

DOE and its 17 national laboratories are uniquely positioned to develop AI capabilities for the nation, leveraging key enabling components:

Data: DOE is the leading generator of classified and unclassified scientific data through the world's largest collection of advanced experimental facilities, including particle accelerators, powerful light sources, specialized facilities for genomics and nanoscience, and neutron scattering sources.

Computing: For decades, DOE has built and operated the world's fastest, most powerful, and highly energy efficient supercomputers. These supercomputers are strategic components of the nation's defensive capabilities, drive innovation through open access to the scientific community, and are the basis upon which to build safe and trustworthy AI capability for the nation.

Workforce: DOE and its national labs host over 40,000 physicists, chemists, biologists, materials scientists, and computer scientists, who tackle some of the most urgent challenges in the national interest.

Partnerships: DOE has unparalleled experience in mission-driven public-private collaborations. Through the Exascale Computing Project (ECP), DOE worked with industry partners to co-design and develop critical components of the computer chips that power today's leading AI models.

The proposed Frontiers in AI for Science, Security, and Technology (FASST) initiative leverages DOE's enabling infrastructure to deliver key assets for the national interest:

Advance National Security. The development of AI models for national security applications, such as threat detection and strategic deterrence is crucial to maintaining America's defensive posture.

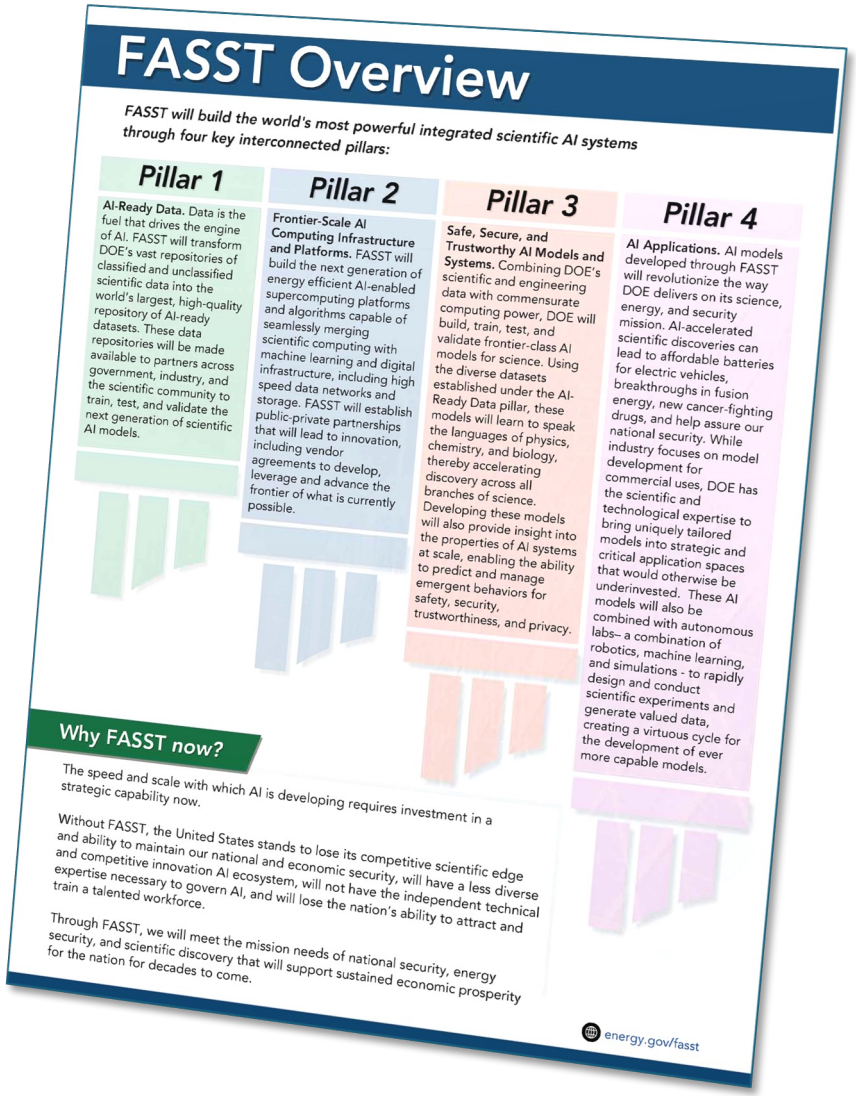
Attract and build a talented workforce. FASST is the most ambitious AI initiative of its kind. This mission will attract, train, and retain top scientific talent for a leading capability deployed in the public interest.

Harness AI for Scientific Discovery. FASST will develop AI tools that will dramatically reduce the time to discovery and extend the nation's competitive edge in technological innovation.

Develop technical expertise necessary for AI governance. FASST will provide insight and independent expertise to quickly inform and validate standards and regulations for a responsible and safe AI industry.

Address Energy Challenges. FASST will unlock new clean energy sources, optimize energy production, and improve grid resilience, and build tomorrow's advanced energy economy. America needs low-cost energy to support economic growth and FASST can help us meet this challenge.

VER. 1.0 JULY 2024



FASST Overview

FASST will build the world's most powerful integrated scientific AI systems through four key interconnected pillars:

Pillar 1

AI-Ready Data. Data is the fuel that drives the engine of AI. FASST will transform DOE's vast repositories of classified and unclassified scientific data into the world's largest, high-quality repository of AI-ready datasets. These data repositories will be made available to partners across government, industry, and the scientific community to train, test, and validate the next generation of scientific AI models.

Pillar 2

Frontier-Scale AI Computing Infrastructure and Platforms. FASST will build the next generation of energy efficient AI-enabled supercomputing platforms and algorithms capable of seamlessly merging scientific computing with machine learning and digital infrastructure, including high speed data networks and storage. FASST will establish public-private partnerships that will lead to innovation, including vendor agreements to develop, leverage and advance the frontier of what is currently possible.

Pillar 3

Safe, Secure, and Trustworthy AI Models and Systems. Combining DOE's scientific and engineering data with commensurate computing power, DOE will build, train, test, and validate frontier-class AI models for science. Using the diverse datasets established under the AI-Ready Data pillar, these models will learn to speak the languages of physics, chemistry, and biology, thereby accelerating discovery across all branches of science. Developing these models will also provide insight into the properties of AI systems at scale, enabling the ability to predict and manage emergent behaviors for safety, security, trustworthiness, and privacy.

Pillar 4

AI Applications. AI models developed through FASST will revolutionize the way DOE delivers on its science, energy, and security mission. AI-accelerated scientific discoveries can lead to affordable batteries for electric vehicles, breakthroughs in fusion energy, new cancer-fighting drugs, and help assure our national security. While industry focuses on model development for commercial uses, DOE has the scientific and technological expertise to bring uniquely tailored models into strategic and critical application spaces that would otherwise be underinvested. These AI models will also be combined with autonomous labs– a combination of robotics, machine learning, and simulations - to rapidly design and conduct scientific experiments and generate valued data, creating a virtuous cycle for the development of ever more capable models.

Why FASST now?

The speed and scale with which AI is developing requires investment in a strategic capability now.

Without FASST, the United States stands to lose its competitive scientific edge and ability to maintain our national and economic security, will have a less diverse and competitive innovation AI ecosystem, will not have the independent technical expertise necessary to govern AI, and will lose the nation's ability to attract and train a talented workforce.

Through FASST, we will meet the mission needs of national security, energy security, and scientific discovery that will support sustained economic prosperity for the nation for decades to come.

energy.gov/fasst

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Data

Scientific & Engineering Datasets

Mathematics
Biology
Materials
Chemistry
Particle Physics
Nuclear Physics
Computer Science
Climate
Medicine
Cosmology
Fusion Energy
Accelerators
Reactors
Energy Systems
Manufacturing

Text and Code Corpora

General Text
Media
News
Humanities
History
Law
Digital Libraries
OSTI Archive
Scientific Journals
arXiv
Code repositories
Data.gov
PubMed
Agency Archives

DOE and NNSA Exascale Systems
FASST Common AI Software Frameworks
FASST Responsible AI Techniques

Compute

Training

Training

Models

Open Science Foundation Models

National Security Foundation Models

Integrated Research Infrastructure
Online Experimental Facilities
Strategic Partnerships

Applications

Tuned and Adapted Downstream Models

Exemplar DOE Mission Tasks

Scientific Discovery

Digital Twins

Inverse Design

Code Optimization

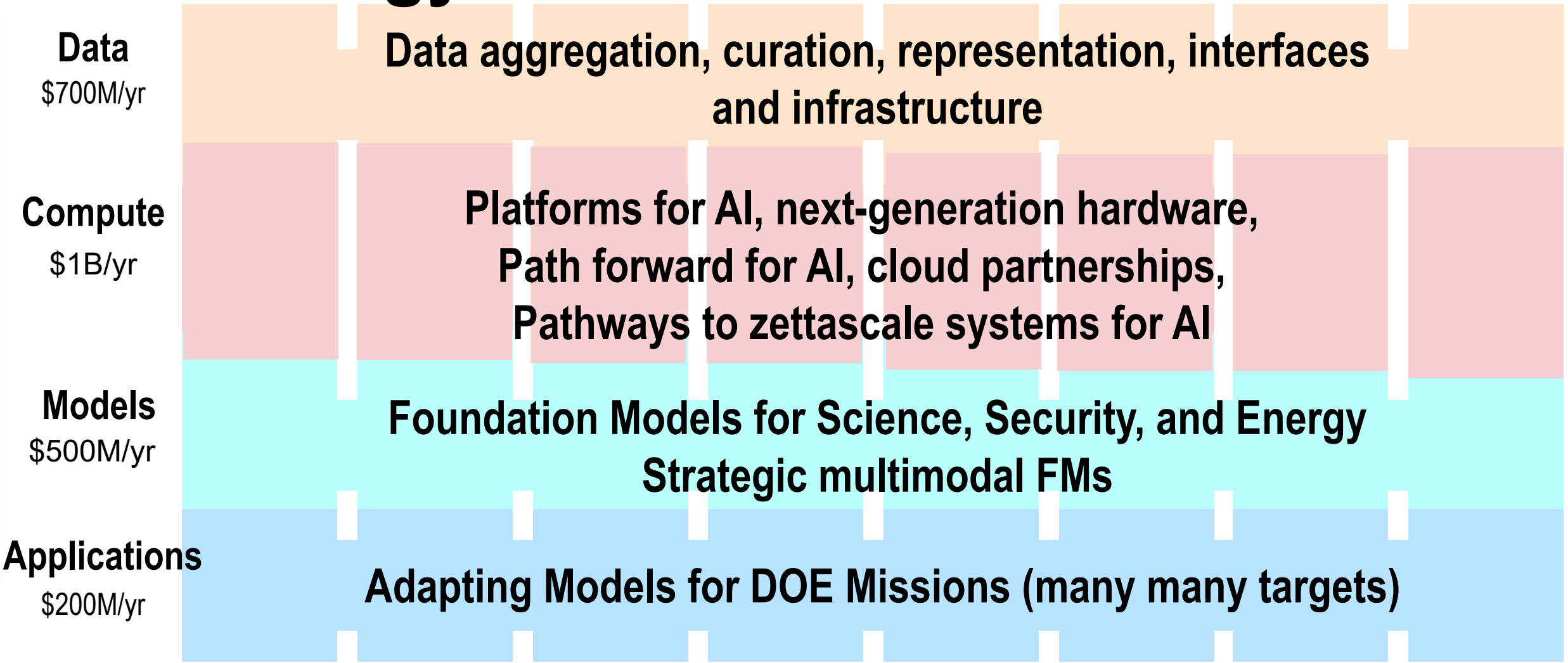
Accelerated Simulations

Autonomous Experiments

Secure Data Infrastructure

Co-Design

Frontier AI for Science, Security, and Technology



Foundation Models Mapped Against DOE Mission Areas

Clean Energy Systems Model: This model would focus on the physics, chemistry, and engineering principles underlying various renewable energy sources, hydrogen production, solar energy, wind energy, and storage technologies. It can be fine-tuned for specific energy systems, optimization of energy output, and efficiency improvements.

Smart Grid and Infrastructure Model: This model would encompass electrical engineering, network optimization, smart grid technologies, and energy systems management. It can be fine-tuned for specific applications like EV infrastructure planning, grid resilience strategies, and smart grid implementations.

Computational Intelligence Model: This model would integrate capabilities in high-performance computing, machine learning, quantum algorithms, computer science, mathematics, computer architecture, data science, advanced data analysis, applied mathematics, and parallel computing. It can be fine-tuned for applications in AI, complex simulations, and computational research.

Environmental Sciences Model: This model would focus on climate modeling, environmental impact assessments, atmospheric science, climate mitigation strategies, climate risk assessment, bio-geosphere interactions, climate engineering, and biological systems in the environment. It can be fine-tuned for specific environmental applications and climate studies.

Materials and Chemical Sciences Model: This model would cover computational chemistry, materials discovery, molecular dynamics, manufacturing processes, inverse design of materials and systems, self-driving laboratories, and autonomous discovery. It can be fine-tuned for developing new materials, chemical processes, and manufacturing techniques for energy applications.

Biological Systems Model: This model would cover the study of biological systems, including genomics, synthetic biology, microbiology, environmental biology, engineering plants, medicine, protein design, self-driving laboratories, autonomous discovery, and microbial engineering. It can be fine-tuned for applications in environmental biology, plant engineering, biotechnology, and medical research.

Nuclear Security Model: This model would integrate nuclear physics, engineering, security protocols, reactor technologies, nuclear fission, automated reactor design, and reactor control. It can be fine-tuned for nuclear energy applications, nonproliferation technologies, and national security measures.

High-Energy and Particle Physics Model: This model would focus on the principles of high-energy physics, nuclear reactions, particle physics, accelerators, and cosmology. It can be fine-tuned for applications in experimental physics, particle accelerators, and fundamental research in physics.

Advanced Manufacturing Model: This model would focus on manufacturing technologies, including inverse design, process optimization, supply chain optimization, applied materials, precision manufacturing, self-driving laboratories, and autonomous discovery. It can be fine-tuned for specific applications in optimizing manufacturing processes and supply chains.

Carbon Management Model: This model would integrate knowledge on the physics and chemistry of capturing CO2, managing CO2 flows, carbon storage, conversion to fuels, and direct air capture. It aims to support the design and analysis of CO2 management systems and advance research into the fundamentals of carbon management.

Knowledge Integration Model: This model would integrate scientific literature, codes, texts, and tutorials to support knowledge extraction, synthesis, and automated hypothesis generation. It aims to advance theory and experimental design, forming the core of a system that interacts with humans and manages interactions with other foundation models included in this list.

FASST Goals and Outcomes

- Ensure US (DOE) **leads the world in technical capability** for its missions in Science, Energy and National Security
- **Create, deploy and sustain world leading ”frontier” AI systems** and **applications** for DOE mission areas to provide advantage to US and partners
- Increase productivity and capabilities of the **DOE laboratories, academic, agency and international partners**
- Develop an **AI-forward workforce** for DOE

- **Discovery Science** – accelerate and improve effectiveness
- **Energy Transition** – accelerate, reduce risk, improve translation
- **National Security** – anticipate risk, mitigate risks, accelerate mission

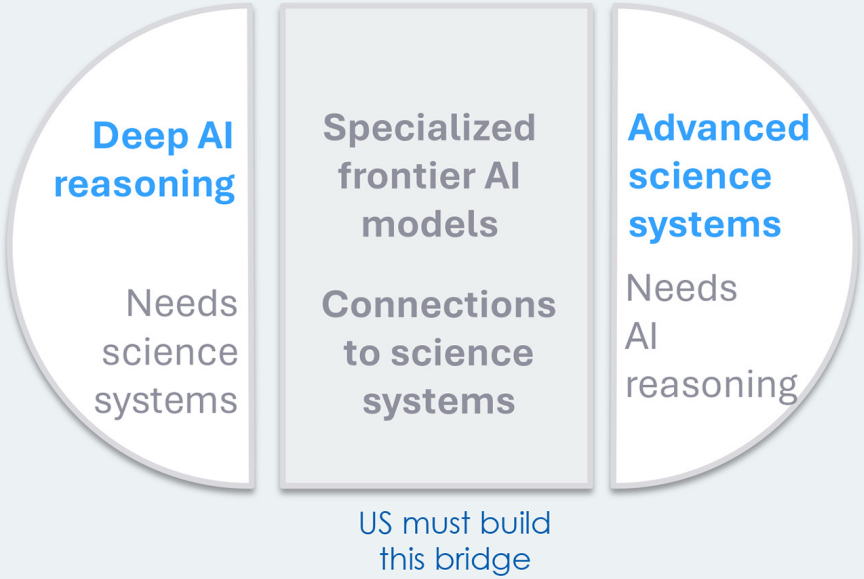
We Must Re-Think Deeply the Industry and Lab Roles

DOE starts where industry stops

From Brian Spears, LLNL Presentation@G17

Industry AI

Best reasoning models



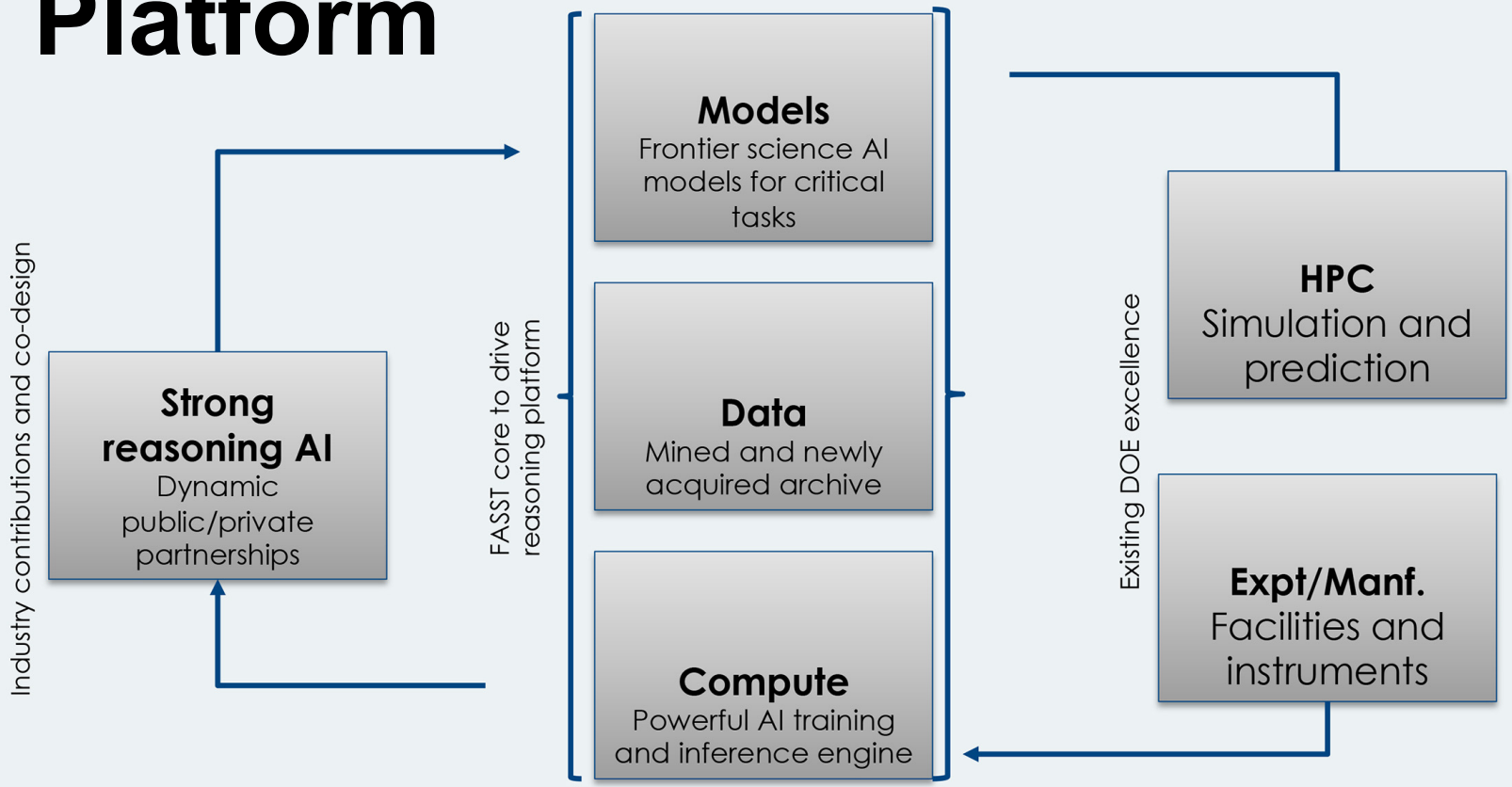
Laboratory science

Most challenging tasks

- AI industry roles
  - Bring the *latest advances in reasoning and planning* technologies
  - Contribute to development of deep expert tools with the labs
  - Collaborate on development of independent safety-security processes and technologies
  - Advance models based on increasingly challenging tasks and problems

- Lab roles
  - Learn to integrate reasoning and learning into larger-scale complex workflows
  - Bring challenging problems, tasks, and data
  - Focus on *Deep expert tools with AI*, physics-based simulation, and unique experimental tool
  - Collaborate on development of independent safety-security processes and technologies

National Investment Should Produce a First-of-its-Kind, Large-scale Scientific Reasoning Platform



Platform capability

1. AI-driven HPC use
2. AI-driven facility use
3. Closed loop for acting on edge data
4. Automated reasoning and hypothesis exploration
5. Accelerated discovery of novel science and solutions

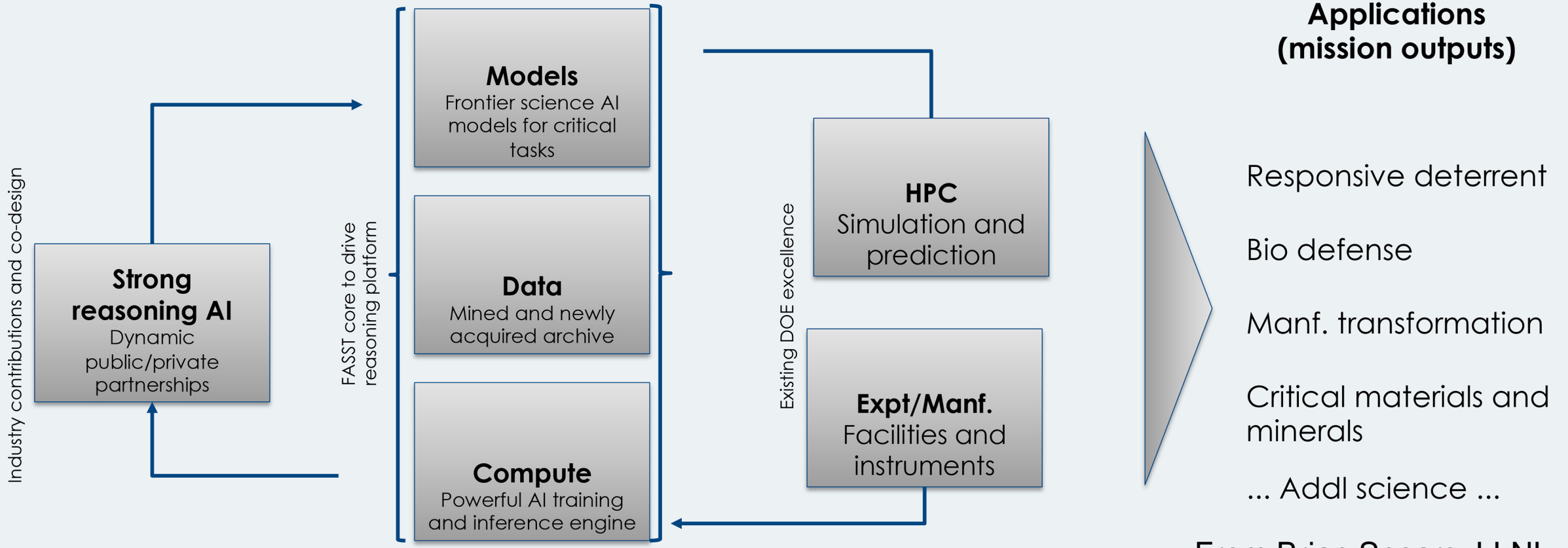
Increasing integrated technical maturity

A closed-loop accelerated scientific reasoning platform (fundamental AI research)

Brookhaven National Laboratory

From Brian Spears, LLNL Presentation@G17

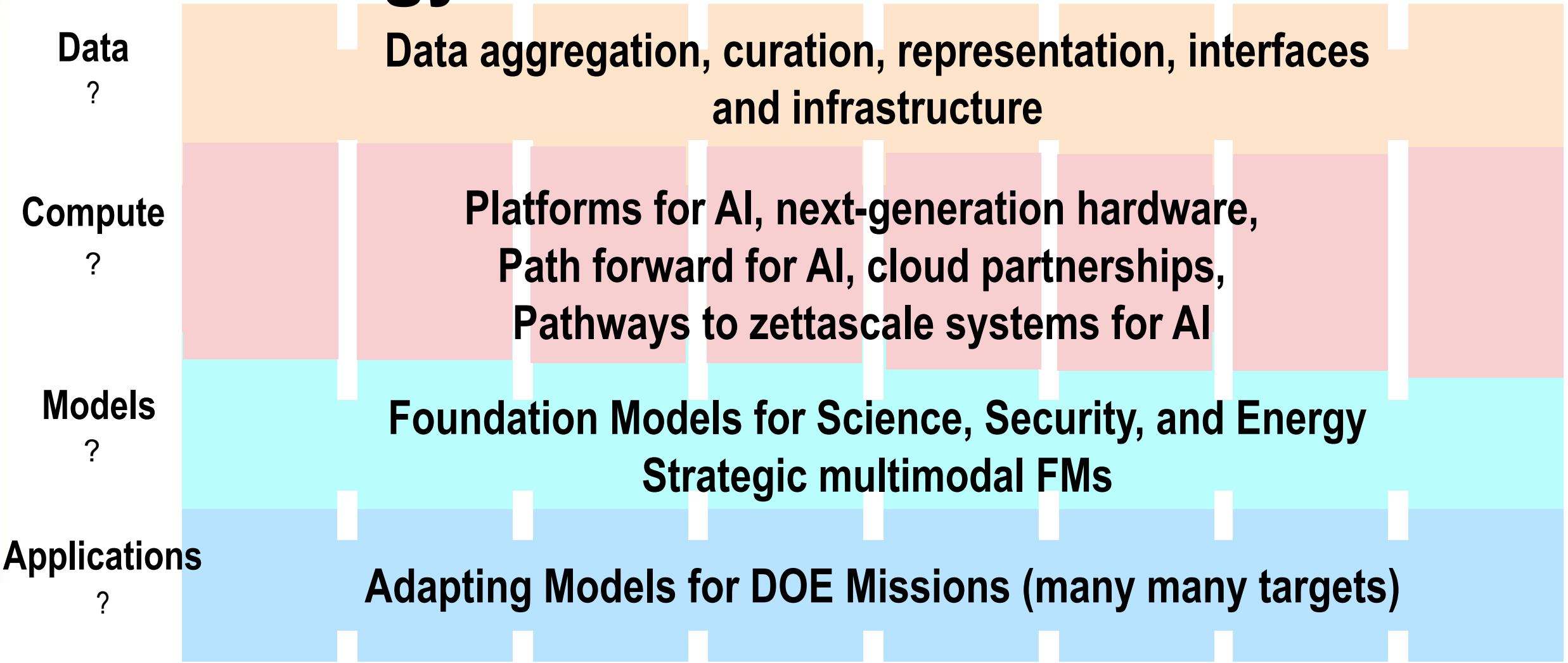
The Platform will Deliver Our Most Critical Application Results



A closed-loop accelerated scientific reasoning platform

From Brian Spears, LLNL Presentation@G17

Frontier AI for Science, Security, and Technology



Elements of a FASST 2.0 concept (*AI):

Foundations of Science and Technology:

- Combating nuclear threats
- Developing advanced deterrence technologies
- Achieving new era of US energy leadership
- Anticipating and neutralizing biological threats
- Creating materials, chemicals, new technologies for national security
- Accelerating basic science

Elements of advanced Ai strategy:

1. DOE scientists have first class access to leading edge AI models
2. Develop a set of challenge problems – DOE's aspirational use cases of advanced AI
3. Assess current commercial AI performance against DOE challenges (including for prioritizing investments in the 4 pillars)
4. Significant expansion of computing capabilities: co-design for energy efficiency, performance and reliability – work with vendors
5. New partnership models with industry and academia

1000 Scientists Jam Sessions

- Access to leading foundation models with reasoning capabilities
- First session on February 28th: BNL will be a hosting site!
- OpenAI's leading model (could be O3!!) will be the first model to be utilized
- Application and selection process
- Problem selection and AI proficiency are pre-requisites
- Planning moving at the speed of AI progress, got to get ready on a very short fuse

Some details

Key Research Question

To what degree (if any) is the use of ‘reasoning’ models likely to improve research and development productivity across the National Labs (and by extension the US scientific ecosystem)?

Sub Questions:

- Are productivity gains (if any) likely to differ across different domains of science?
- Are productivity gains (if any) likely to differ across different categories of tasks within research & development?
- What additional capabilities (underlying performance, UI changes, additional features etc.) are most likely to improve the utility of these models for science (based on the Jam specifically)?

Data will need to be gathered in such a way as to isolate the following variables related to model performance:

1. Model ‘world knowledge’ e.g. what it has already memorized
2. Model ‘additional knowledge’ e.g. quality of RAG or provided additional data
3. Model ‘reasoning’ e.g. the ability to generate novel information from inputs + data + prompts
4. Prompt quality e.g. testing variations of each prompt on quality of answer

Research Problem Selection

The use of ‘telescoping’ problem is recommended: breaking research into ascending orders of complexity and domain/technical specificity.

Example: Isolating Key Variables for Fusion Reactor Design

The end goal here could be getting the model to try and generate novel reactor designs in order to accommodate ever more specific - and interrelated - variables. To achieve that the telescoping order might be something like:

- Baselining what the models know innately about the theory of fusion
- Baselining how up to date the models are about existing reactor designs + experiments
- Providing additional data and assessing how that changes model answer
- Prompting the model to list what variables are significant + why they are significant
- Deep diving into a specific variable to assess model understanding of individual cause and effect
- Asking the model to represent that cause and effect in mathematical terms etc.
- Pushing model extrapolation based on that individual variable
- Repeating the process for other impactful variables
- Repeating the process for multiple variables and the emergent complexity produced
- Asking the model to provide a recommendation / design output / mathematical model to summarize the work done for further refinement

Logistics

Registration

Teaming

Reporting

Analysis

More events like this one to come