AI for Science, Energy and Security

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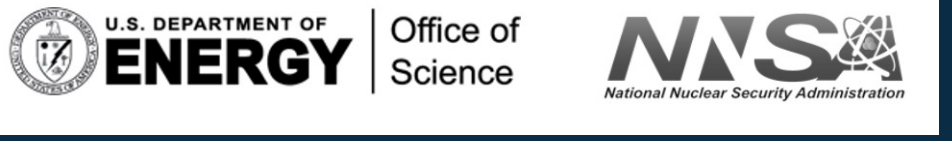
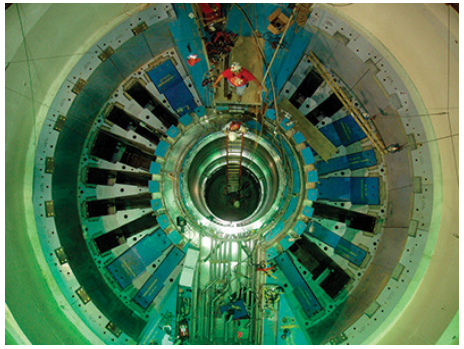
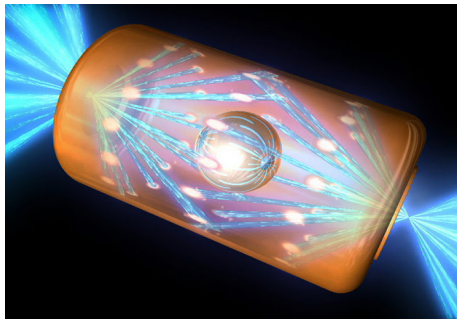


DOE's Unique Position for AI Leadership

- **Operates the most capable computing systems and the world's largest collection of advanced experimental facilities**
- Responsible for US nuclear security through deep partnerships across government
- **Largest producer of classified and unclassified scientific data in the world**
- Strongest foundation combining physical, biological, environmental, energy, mathematical and computing sciences
- **Largest scientific workforce in the world**
- Strong ties with private sector technology and energy organizations and stakeholders

World's best experimental facilities and supercomputers




DOE Has Been Gathering Wide Community Input (>1300 researchers)

2019

What changed in three years?

- Language Models (e.g. ChatGPT) released
- Artificial image generation took off
- AI folded a billion proteins
- AI hints at advancing mathematics
- AI automation of computer programming
- Explosion of new AI hardware
- AI accelerates HPC simulations
- AI accelerates HPC simulations
- Exascale machines start to arrive

2022

2020 DOE Office of Science ASCR Advisory Committee report recommending major DOE AI4S program

Report posted here:
https://www.anl.gov/ai-for-science-report

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Workshops organized on six crosscutting themes

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, Assured AI for scientific knowledge

Hypothesis Formation, Math
Theory and Modeling Synthesis,

Let’s look at one* example theme

*Many detailed examples are in the report

And in the backup slides at the end of this deck

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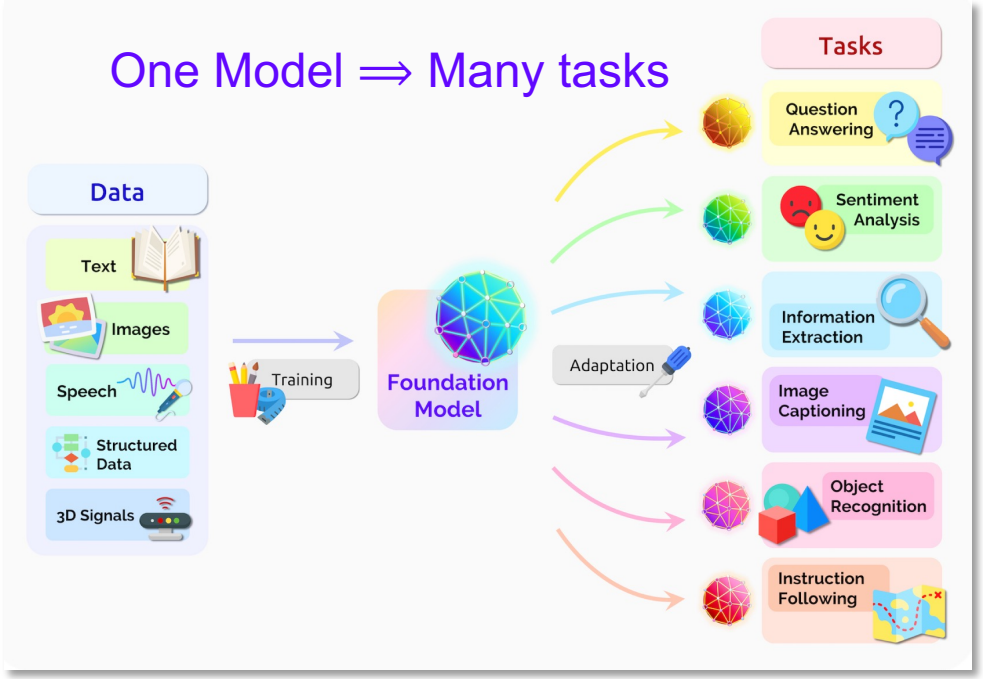
Foundation Models — What are they?

- **Large scale model trained on large datasets from many sources** (text, papers, datasets, code, molecules, etc.)
- **Additional training to improve the human interaction experience** (e.g., ChatGPT-4)
- **Large models are remarkably flexible and exhibit emergent behaviors** (capable of tasks not originally trained to do)
- **Many hundreds of applications built on top**
- There are early efforts underway in DOE labs to create Foundation Models explicitly targeting scientific discovery

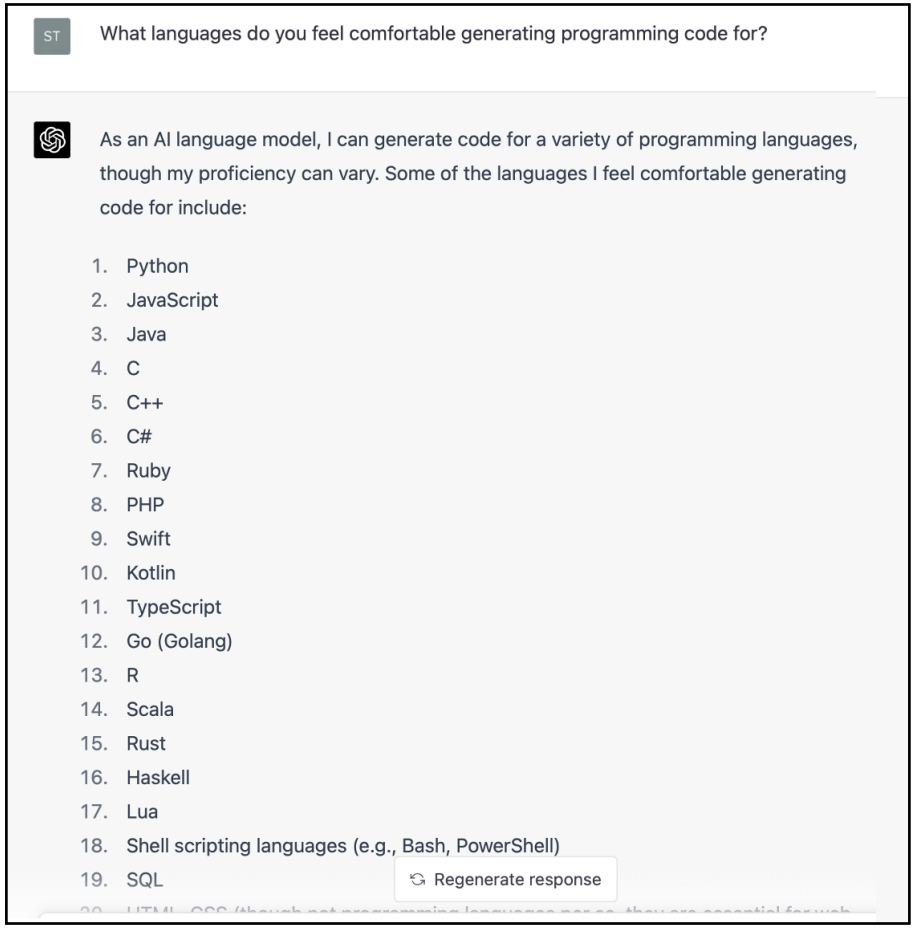


Trained on trillions of input ”tokens”
for many weeks on a large-scale computers

SOTA models (GPT-4) have about
1 trillion parameters (1% brainscale)

Foundation Models – Opportunities

- **FMs can summarize and distill knowledge** – extract information from million of papers into compact computing representation – PPI networks, materials compositions, code kernels, biological function, etc.
- **FMs can synthesize** – combine information from multiple sources – generate small programs for specific tasks – quantum computing programs using QISkit & Cirq, derivations for applied physics, code for visualization and animation, etc.
- **FMs can generate plans, solve logic problems** and write experimental protocols for robots – powering self-driving labs, generate strategies for problem solving, and planning for testing hypotheses



Foundation Models — Current State

- **Very rapid progress since 2019:** Foundation Models are the closest things that have yet been created that hint at the possibility of Artificial General Intelligence
- **FMs need additional research to generate useful, verifiable hypotheses and theories for exploration – but** a full-time shared scientific assistant that learns from across all of science is appears to be possible

"After experimenting with GPT-4 in our own research domains in materials chemistry, physics and quantum information, we find that ChatGPT-4 is knowledgeable, frequently wrong, and interesting to talk to. In other words, not unlike a college professor or a colleague" https://arxiv.org/pdf/2304.12208.pdf

Fundamental and applied foundation model research is needed for trusted, assured AI models in DOE

Can ChatGPT be used to generate scientific hypotheses?

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Abstract

We investigate whether large language models can perform the creative hypothesis generation that human researchers regularly do. While the error rate is high, generative AI seems to be able to effectively structure vast amounts of scientific knowledge and provide interesting and testable hypotheses. The future scientific enterprise may include synergistic efforts with a swarm of "hypothesis machines", challenged by automated experimentation and adversarial peer reviews.

In a university or research institute, a significant portion of fresh ideas arises out of discussions. Can talking to ChatGPT-4,[1] OpenAI's latest chatbot, create genuinely interesting scientific hypotheses?

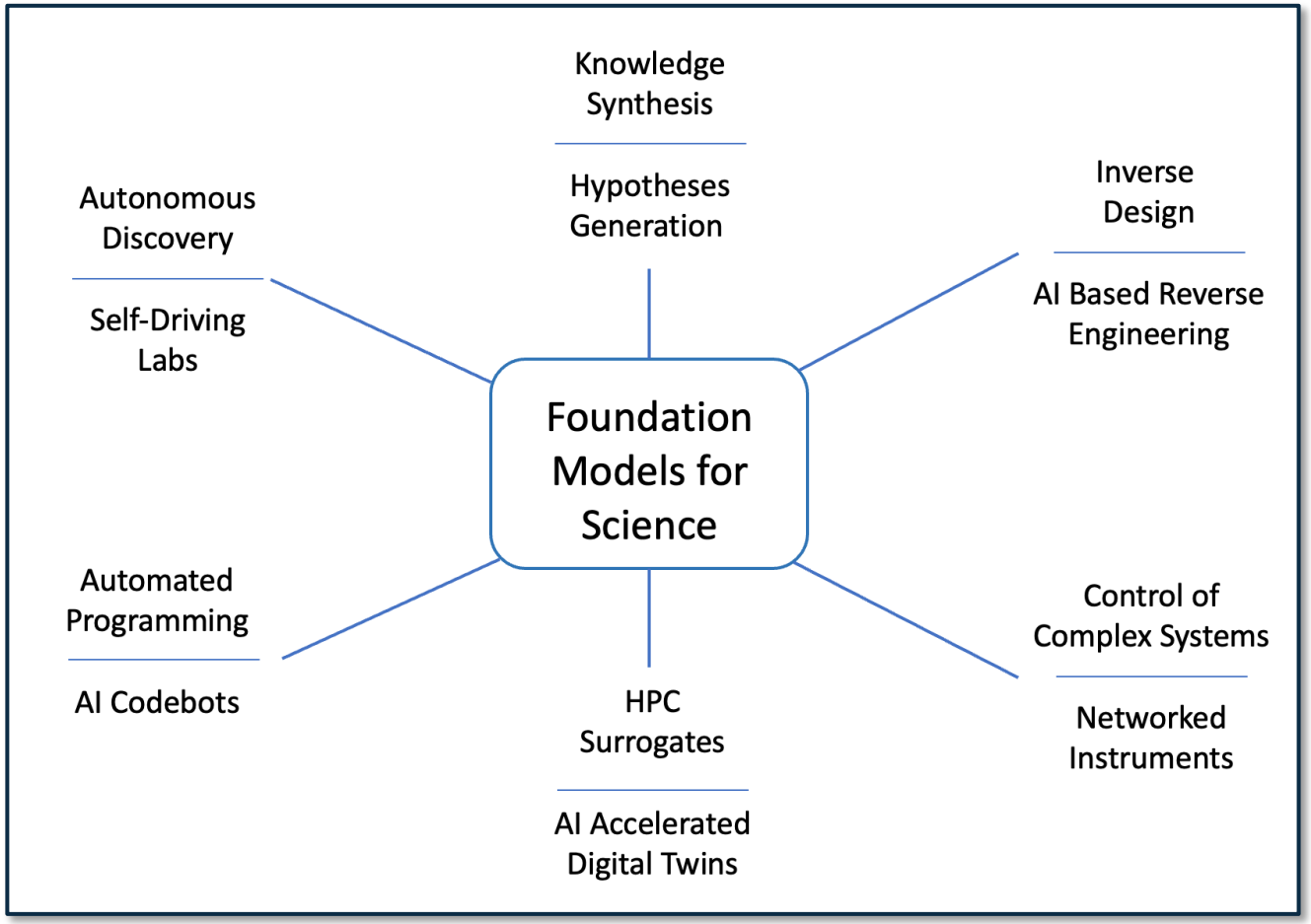
In the past, only humans generated interesting hypotheses. Computers have been used to perform numerical simulations or even to prove theorems, like the four-color theorem in 1976[2]. But making interesting laboratory-testable hypotheses with artificial intelligence (AI) seems far-fetched, until recently.

We are a collaborative group of experimental and theoretical researchers in physical sciences and engineering. Generative Pre-trained Transformer (GPT-4), released on March 14, 2023, is a large language model (LLM) significantly bigger than its predecessor GPT-3 released in 2020 (already with 1.75×10^{11} parameters). GPT-4 neural network was trained on a text corpus of books, webpages, academic papers from various disciplines, discussion forums, etc., up to September 2021. After experimenting with GPT-4 in our own research domains in materials chemistry, physics and quantum information, we find that ChatGPT-4 is knowledgeable, frequently wrong, and interesting to talk to. In other words, not unlike a college professor or a colleague.

To make everything concrete, our operative definition of "genuinely interesting scientific hypotheses" is (a) whether after a conversation, some experienced practitioner of a field can feel

1

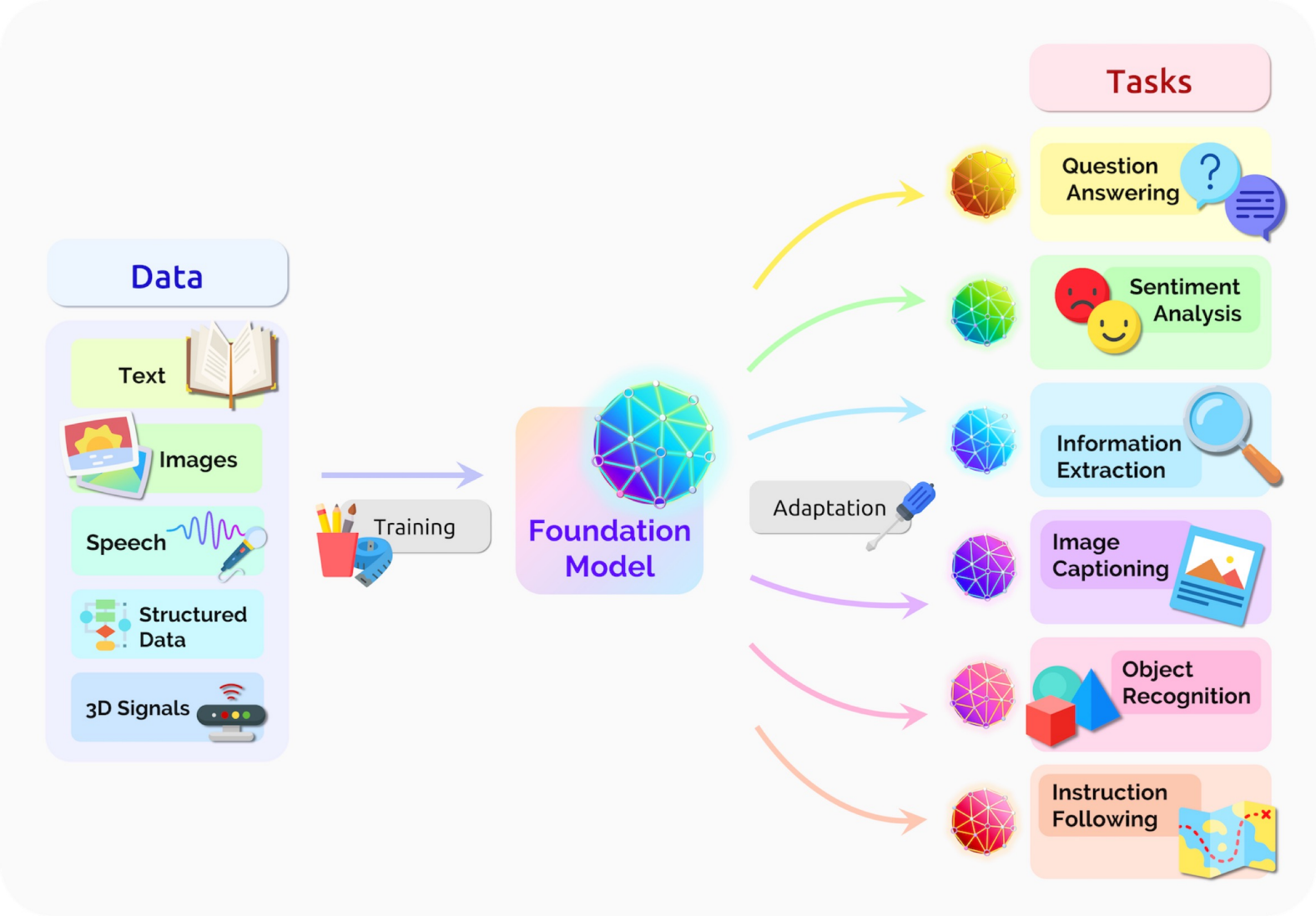
It is possible that many of the use cases we imagine in the AI4SES report can be driven directly or indirectly from sufficiently powerful Foundation Models



Leveraging Community Efforts

Scientific & Engineering Datasets

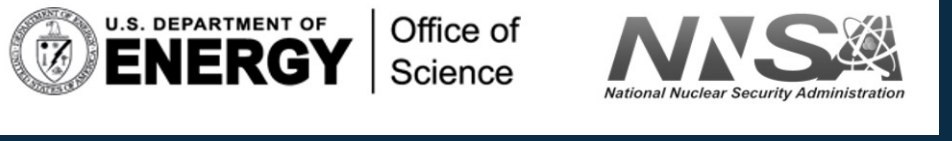
Mathematics
Biology
Materials
Chemistry
Particle Physics
Nuclear Physics
Computer Science
Climate
Medicine
Cosmology
Fusion Energy
Accelerators
Reactors
Energy Systems
Manufacturing



Exemplar DOE Mission Tasks

- Scientific Discovery
- Digital Twins
- Inverse Design
- Code Optimization
- Accelerated Simulations
- Autonomous Experiments
- Secure Data Infrastructure
- Co-Design

Workshop meetings elucidated major opportunities for AI-enabled technologies and solutions to time-sensitive DOE mission challenges



Exemplars where AI plays a transformative role

Science

- Safe control a fusion reactor to sustain long plasma burns
- Porting scientific codes for new computer hardware without human intervention
- Accelerated and automatic interpretation of data from particle detectors

Energy

- Optimization of product designs and manufacturing processes
- Predictive models for energy output from variable/uncertain energy sources
- Next-generation energy-efficient microelectronics

Security

- Accelerating design and analysis for modernizing the nuclear deterrent
- Accelerating certification time and reducing manufacturing costs
- Expands options for addressing evolving national security threats

Responsible AI R&D is needed to Execute Our Science, Energy and Security Missions

General Society AI Risks

- Disinformation and Deepfakes
- Surveillance and Privacy Violations
- Social and Behavioral Engineering
- Bias and Discrimination
- Market Manipulation

Global Security AI Risks

- Autonomous and Swarm Weapons
- Biosecurity and Novel Agents
- Nuclear Proliferation
- New Approaches to Chemical Weapons
- Accelerated Cyberwarfare

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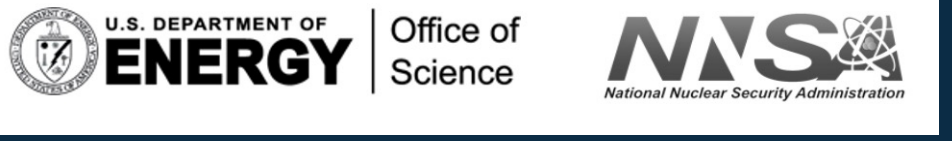
DOE is well positioned to be a leader in the US government for trustworthy and responsible AI R&D

We need to do it for DOE mission space, but the country needs this capability for broader reasons



DOE Can Be A World Leader to Advance Responsible AI Development

- Driven by mission in science, energy and security (e. g. need trustworthy AI for high-consequence national security applications)
- World-leading R&D expertise (e. g. history of large-scale interdisciplinary teams)
- Strong foundation to create AI-enabled solutions (e. g. world's most capable user facilities, NNSA-SC working together to advance computing in a 7-year $1.8B project)
- Uniquely positioned for AI implementation (e. g. strong ties with private sector technology and energy organizations)

Only DOE/NNSA can advance responsible Co-Design of AI R&D with a strong focus on science, energy and national security via simultaneously tying R&D to mission, thereby creating and implementing solutions

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AI4SES builds on previous community input to provide a blueprint to execute a comprehensive DOE-wide effort.

We can leverage our experience with large-scale integrated efforts such as ECP, and Hubs.

Frontiers of AI for Science, Security and Technology

Integrated science R&D on alignment, ethics and responsibility

Transformational hub-scale-centers on key AI4SES themes strong ties to program grand challenges

Crosscutting AI technologies

Dedicated access to computing and experimental facilities