

AI for Science, Energy and Security

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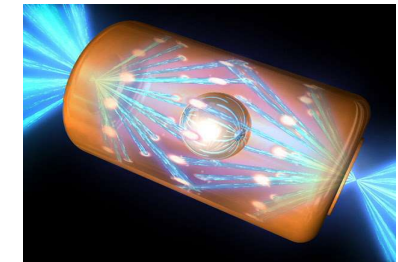
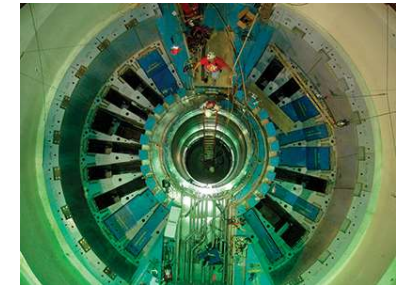
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DOE's Unique Position for AI Leadership

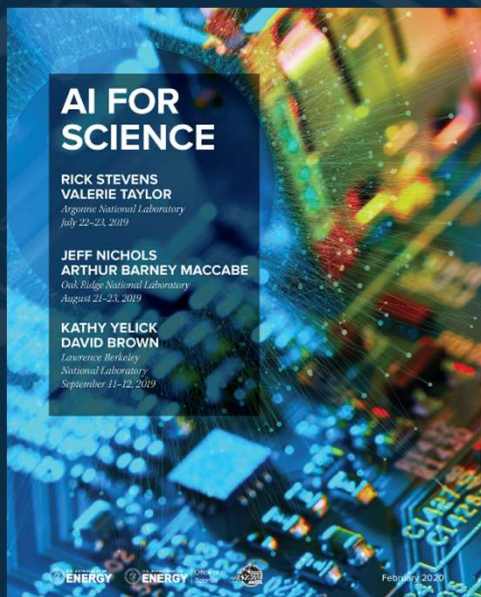
- Operates the most capable computing systems and the world's largest collection of advanced experimental facilities
- Responsible for US nuclear security through deep partnerships across government
- Largest producer of classified and unclassified scientific data in the world
- Strongest foundation 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
- Exascale machines start to arrive

2022



Report posted here:

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

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

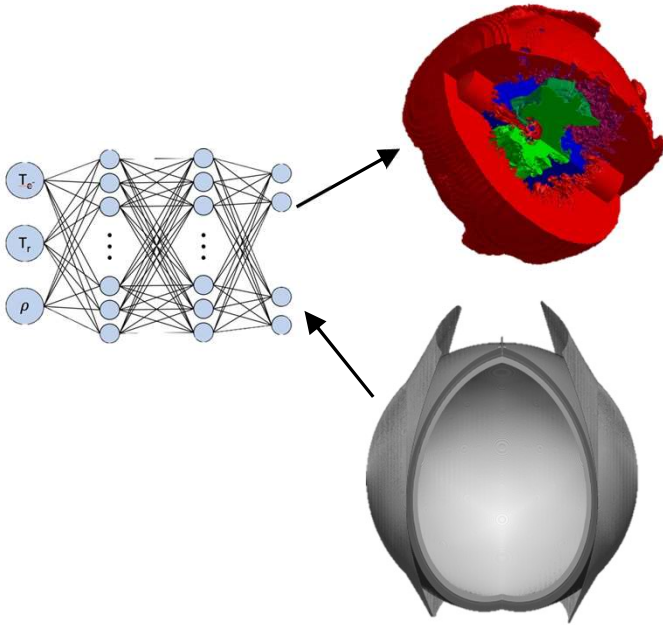


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NNSA
National Nuclear Security Administration

From the workshops it was clear that AI represents a powerful new foundation for progress in science and technology



AI based surrogates for HPC
 Climate Ensembles
 Effective Zettascale on Exa

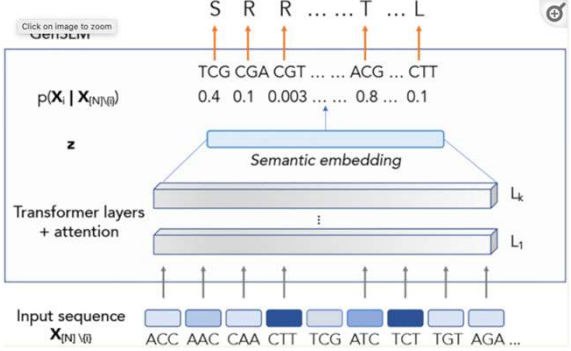
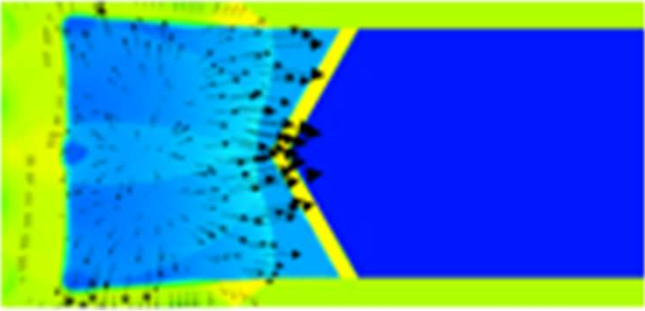
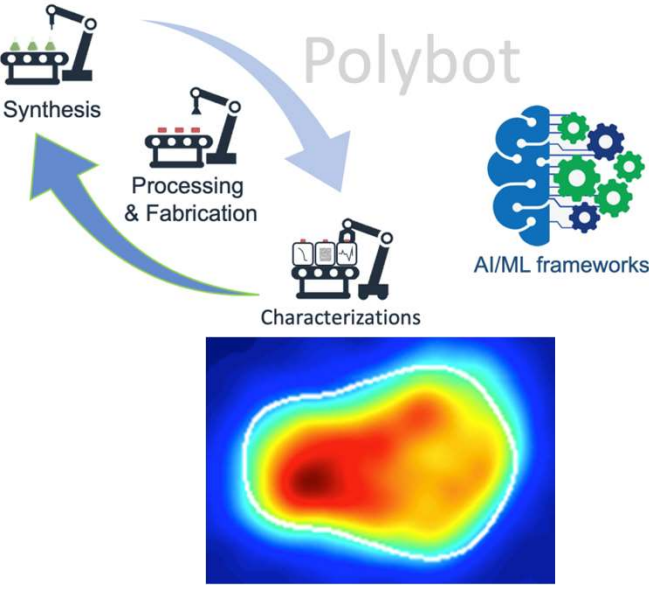
AI and robotics for autonomous discovery
 Materials, Chemistry, Biology
 Light-Sources, Neutrons

AI for software engineering and programming
 Code Translation, Optimization
 Quantum Compilation, QAIgs

AI for prediction and control of complex engineered systems
 Accelerators, Buildings, Cities,
 Power Grid, Networks

AI for advanced properties inference and inverse design
 Energy Storage
 Proteins, Polymers

Foundation AI for scientific knowledge



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



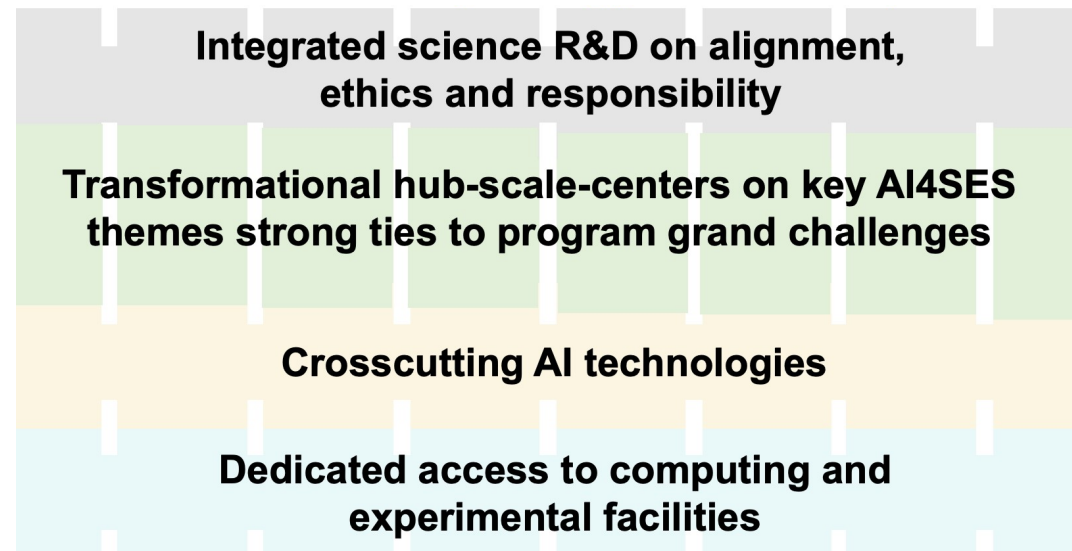
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Realizing the potential of AI for science and security will take a national effort in the tradition of nuclear and high energy physics

- Integrated AI R+D plan supporting data use across science and engineering
- AI computing infrastructure building on DOE's world leading Exascale GPU systems
 - Partner with industry to create new and more energy efficient computing systems
- Unite DOE's user facilities as national platforms that can be AI driven for powerful advances
- A new era of strategic partnerships with universities and international allies



This is now a major international competition. Those using AI will gain asymmetric advantages and displace those who do not.