

Office of High Energy Physics: AI & ML Strategy and Vision

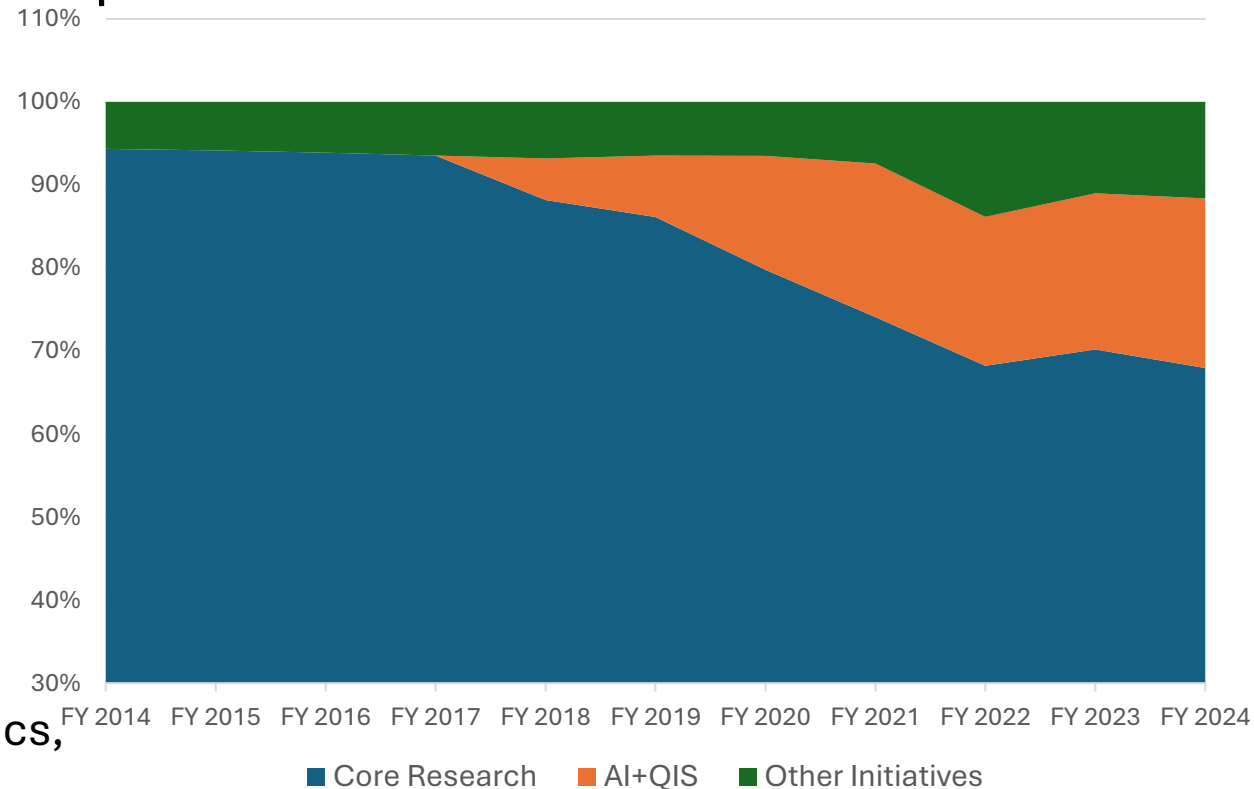
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Office of Science Research Initiatives

- SC Research Initiatives provide focus on areas of strategic importance
 - Initiatives do not change the focus of the HEP mission but emphasize how it can be accomplished with the most impact
- Since 2018, the number of and funding to initiatives has increased
 - In 2017, 93% of DOE HEP's Total Research budget was in Core
 - SBIR/STTR the only non-Core funding
 - In 2024, 69% of DOE HEP's Research budget from appropriation was Core
 - QIS+AI/ML were 20% of total HEP Research
 - All others were 11% combined
 - SBIR/STTR, ASTI, RENEW, Microelectronics, Advanced Computing, Accelerate, FAIR



National Artificial Intelligence Initiative



- February 2019 – [Executive Order to Maintain American Leadership in Artificial Intelligence](#)
 - Key priorities: increase funding for AI research, make use of Federal AI computing and data resources, set AI technical standards, build America's AI workforce, engage international allies
- March 2020 – [National Artificial Intelligence Initiative Act](#) – Codified executive order into law
 - Includes guidance for OSTP to coordinate AI activities across 18 federal agencies, and specific AI responsibilities for NIST (technical standards), NSF (workforce and AI Institutes), and DOE (National AI Advisory Council, workforce, and AI research)
 - Calls for an AI budget roll up across agencies to ensure the research spending is sufficient to accomplish the National AI Initiative goals
- January 2021 – National AI Initiative Office created
- October 2023 – [Executive Order on the Safe, Secure, and Trustworthy Development and Use of Artificial Intelligence](#)
 - Key priorities: safe and secure AI, responsible AI, ethical AI, safeguards to protect Americans from AI, privacy preserving AI, mitigate the risk of government's AI use, AI workforce, and global AI leadership



Role of Science in Oct. 2023 Executive Order

PRESIDENT'S COUNCIL OF ADVISORS ON SCIENCE AND TECHNOLOGY

The President's Council of Advisors on Science and Technology (PCAST) consists of distinguished individuals from sectors outside of the Federal Government who advise the President on policy matters where the understanding of science, technology, and innovation is key.

- April 2024 – [PCAST Report](#) on Supercharging Research: Harnessing Artificial Intelligence to Meet Global Challenges
 - Provides five recommendations for the role scientific research can play in tackling major societal and global challenges laid out in the Executive Order
 - Broadly and equitably share AI resources, secure access to data for critical research needs, basic and applied AI research that involves collaborations across academia and industry, adopt principles of responsible, transparent, and trustworthy AI, encourage integrating AI assistance into scientific workflows

Role of HEP in Oct. 2023 Executive Order

- April 2024 – [PCAST Report](#) on Supercharging Research: Harnessing Artificial Intelligence to Meet Global Challenges
 - The report includes HEP as an example of how interdisciplinary AI research benefits the sciences:

“The cosmologists and particle physicists ... are some of the earliest adopters—and developers—of AI, so an epoch of advanced AI is an epoch of exciting discoveries in fundamental physics and cosmology.”

“Fundamental physics and cosmology are built on statistical analyses of data to test theory, so they require a deep understanding of the probabilities in the interpretation of data. This requirement is driving the mathematical development of AI that can handle probabilistic rigor. ... Assessing uncertainties is crucial for fundamental physics, and probabilistically rigorous AI would be a game changer for many other fields of science as well, in addition to being invaluable for applications beyond science.”

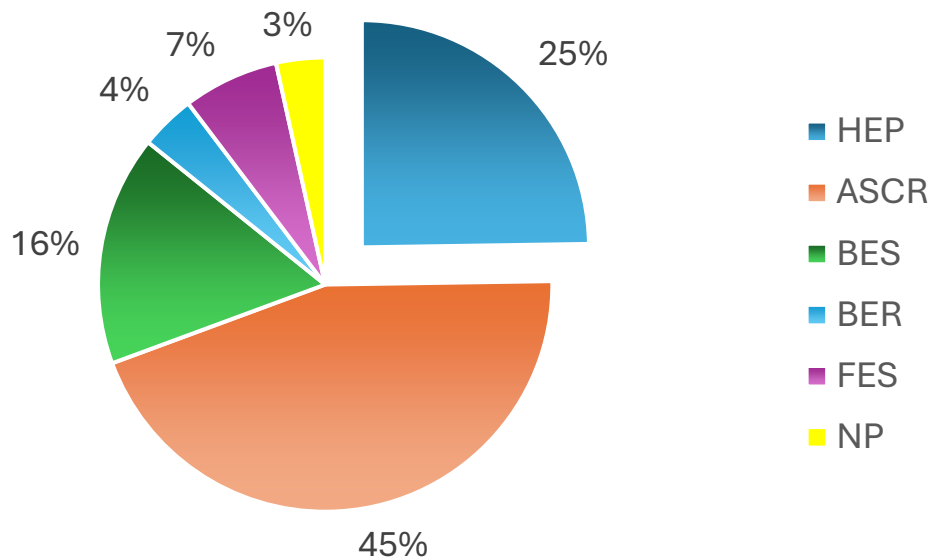
- Not a zero-sum game – HEP relies on AI/ML tools and methods supported outside the particle physics community



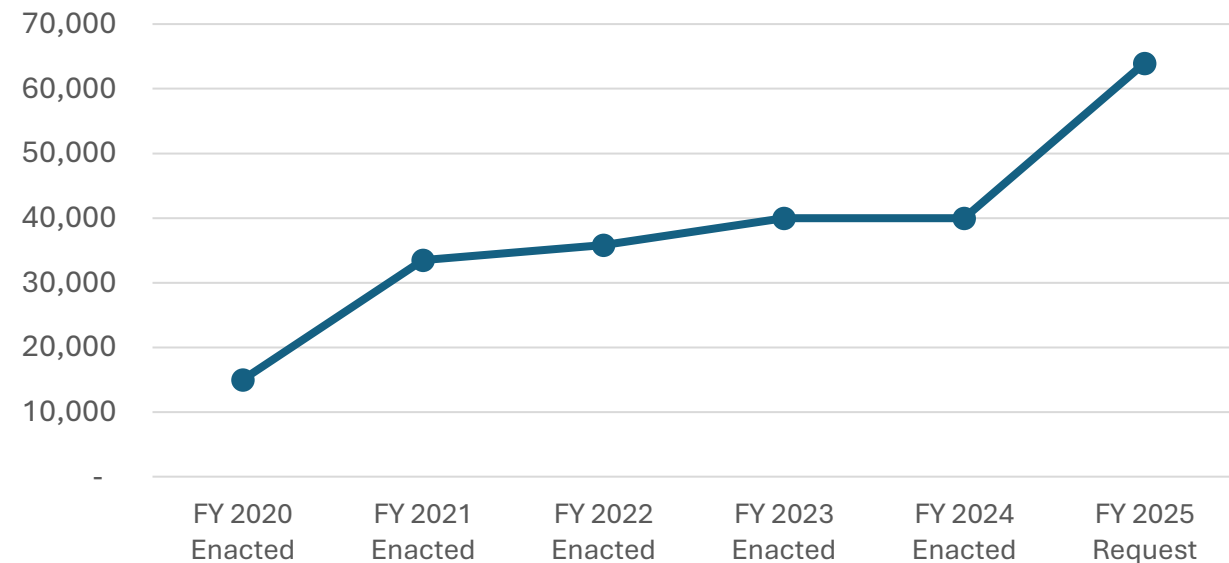
AI/ML Funding at DOE HEP

- SC recognizes the role HEP plays as a data intensive discipline in the AI/ML research ecosystem
 - On average DOE HEP has received 25% of the SC AI/ML Initiative funding
- Since the initiative began HEP AI/ML program has grown \$15M – \$40M
 - President's FY25 Request \$63M

Average Percent of SC AI/ML Funding

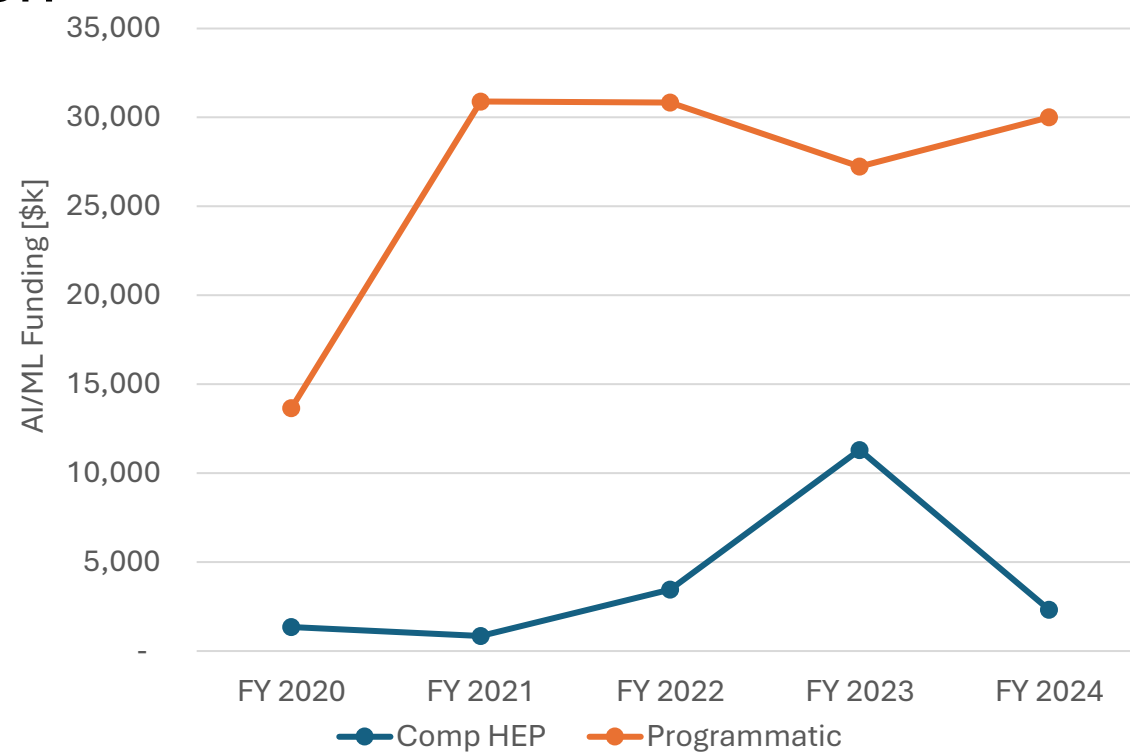


HEP AI/ML Funding [\$k]



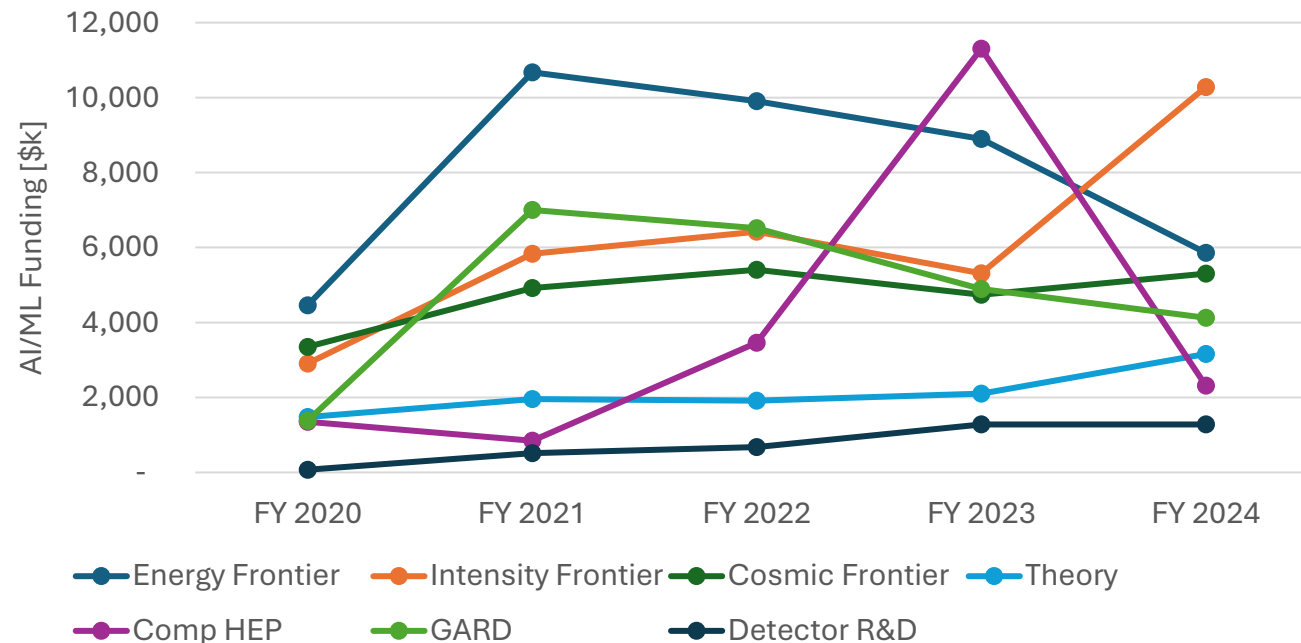
HEP's AI Initiative Implementation

- The 2020 Research Division Committee of Visitors recommended
 - Approval of a hire in AI/ML and HEP Computing. ... A crosscutting strategy for AI/ML and HEP Computing is also a high-priority need.
- DOE HEP has pursued AI/ML research in two distinct thrusts
 - **Programmatic AI/ML** – embedded in the HEP subprograms
 - Approximately 88% of HEP's AI/ML Initiative funding
 - **Core AI/ML** – research to enable future HEP breakthroughs using AI



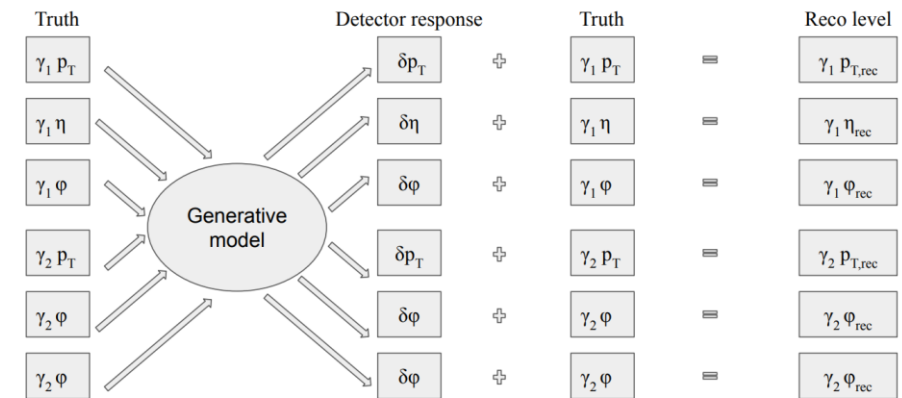
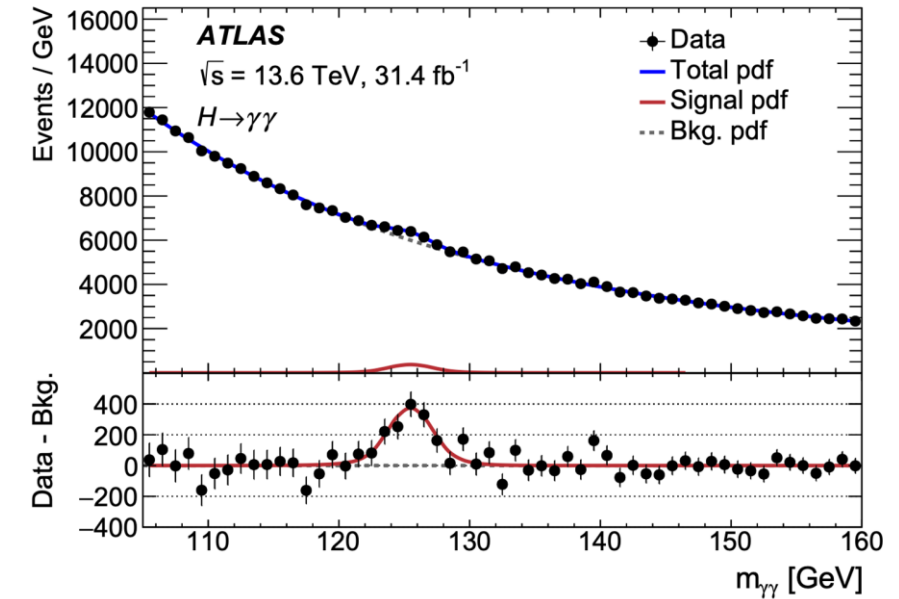
Programmatic AI/ML Research

- Research that furthers the goals of the HEP subprograms
 - Research where the primary benefit is to address existing technical challenges using ML
- Programmatic AI/ML Research is supported as a part of all HEP NOFOs
 - Evaluated as part of a subprogram's standard review of Early Career, Comparative Review (Open Call), US/Japan, etc.



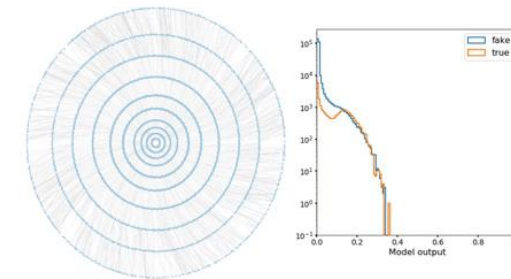
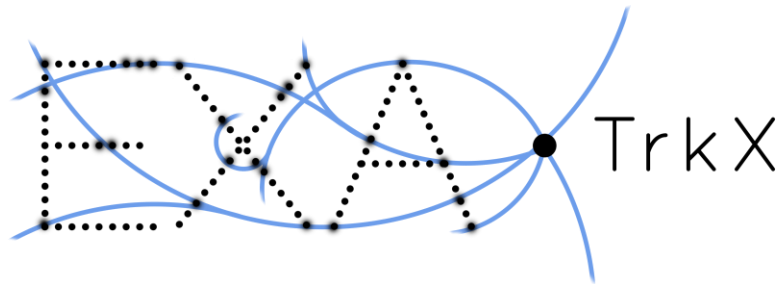
Generative Machine Learning for Detector Effect Modeling

- Generative ML model used in the ATLAS Run-3 Higgs to diphoton measurement
 - Trained with ATLAS simulation samples to learn simulated detector response
 - Applied to $O(100\text{M})$ generator diphoton background events to obtain expected detector response
 - Used to determine the background PDF in the ATLAS paper
 - [Eur. Phys. J. C 84 \(2024\) 78](#)
- Normalizing flows as a generative ML model developed as surrogate for full detector simulation
 - Capture detector response specific to object kinematics and event conditions, model non-Gaussian effects, reproduce correlations between measurements of different objects
 - [JINST 19 \(2024\) 02, P02003](#)



Core AI/ML Research

- Objective of the DOE HEP's Core AI/ML is to realize the potential of AI/ML to benefit HEP's mission
 - Support the full development cycle of advanced AI applications
 - Blue-sky R&D into new methods and techniques relevant to HEP problems
 - Standardized benchmark datasets to allow meaningful comparison between results
 - Transfer R&D into community tools and applications
 - Broaden participation to increase the impact of AI/ML advancements
 - Through maintenance, optimization, and refinement of existing ML applications with increasingly powerful methods and techniques
 - Leverage technical development supported beyond DOE HEP: SC, federal funding agencies, international partners, and industry



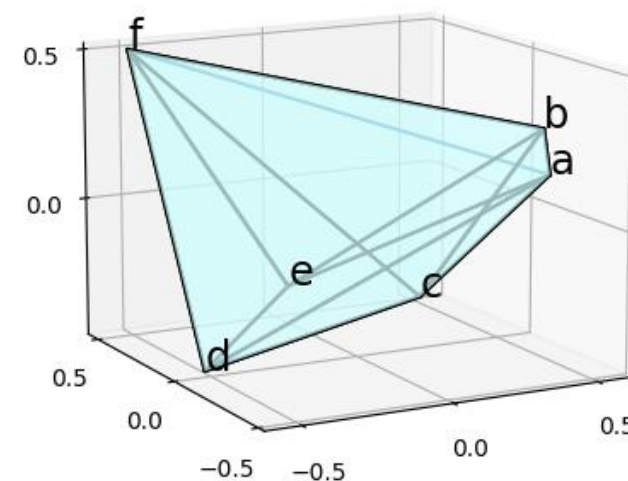
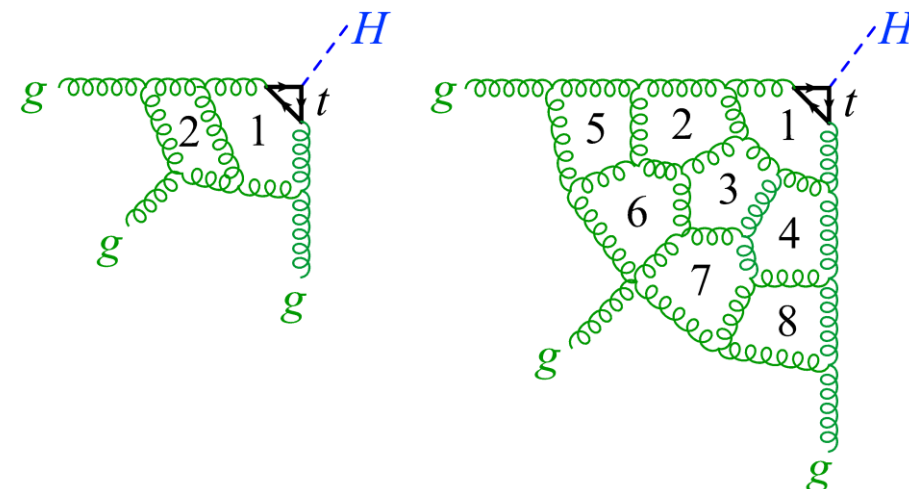
Core AI/ML Program Execution

- Primary sources of Core AI/ML funding have been dedicated opportunities
 - Priority support for ambitious projects and increased participation in HEP AI research
 - Artificial Intelligence Research for High Energy Physics [FOA](#) FY22
 - Research projects supported at 5 DOE Labs and 20 Universities
 - Hardware-Aware AI for HEP [Research Review](#) FY25
 - Review on going
 - AI For HEP Theory and Data Analysis
 - University applications due April 18th through [Open Call NOFO](#) (Lab companion call forth coming)
 - AI Workforce development through DOE HEP Traineeships
 - Supplemental applications due March 31st through [Open Call NOFO](#)
- Beginning in FY24 provide opportunity to build and maintaining a base AI research program
 - Through CompHEP participation in HEP NOFOs
 - Priority support for development that turns productive R&D into community tools and resources and activities in areas of PI's sustained interest

Bootstrapping Transformer Models to Compute Scattering Amplitudes

- Using ML to bootstrap scattering amplitude computation
 - Teach Transformer Models the grammar of Feynman diagrams in *Super Yang Mills* simplified QCD
 - Higher order amplitude terms are predicted with 98% accuracy from training on lower order diagrams
 - R&D towards ML models that can analytically compute scattering amplitudes to arbitrary order
- Research into the fundamental techniques of training a transformer
 - Use Physics knowledge to establish the fundamental dynamics of training transformer networks
 - Model must learn the amplitude term's magnitudes before learning their signs

[Tianji Cai et al 2024 Mach. Learn.: Sci. Technol. 5 035073](#)



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Future Directions

SC AI Roundtables

- This fall the Office of Science held a series of six AI Roundtables
 - Focused on identifying the highest impact research opportunities
 - Each SC AI Roundtable was to identify 3-5 Priority Research Opportunities (PROs) that could guide programs over the next 3-5 years
 - Three Roundtables had significant HEP presence:
 - High Energy and Nuclear Physics, including Accelerator and Instrumentation technology
 - HEP Co-lead Jeremy Love
 - Fabrication Science including Microelectronics
 - HEP POC Helmut Marsiske
 - SC Scientific User Facilities
 - HEP Co-lead Eric Colby and HEP POC Eric Feng
 - Each AI Roundtable was a two-day in-person event with 25-50 participants from across the relevant research communities
 - The HE+NP and Facilities Roundtables distributed surveys to collect input prior to the meetings and used the responses as input to discussions
- The SC Roundtable report is in preparation, expected by mid-2025

HEP Specific AI/ML Planning

- DOE HEP is working with the community to develop HEP-specific AI/ML guidance
 - Engage the community to understand what technical problems AI/ML can have the biggest impact on – Programmatic AI/ML
 - Identify common technical tools, datasets, methods, and challenges that need to be addressed – Core AI/ML
- Extend the SC AI Roundtables findings for a longer 5–10-year vision
 - As possible make the SC AI Roundtable PROs specific to HEP subprograms
- Expect to produce a Basic Research Needs report that will be used to establish DOE HEP's AI/ML research priorities
 - Communicate areas of opportunity and impact to DOE HEP PMs
 - Make clear to HEP researchers the priority AI research topics
- Community engagement is expected to be a component

Conclusion

- SC Initiatives provide emphasis on methods of strategic importance in carrying out the DOE HEP mission
 - The two largest SC Initiatives in HEP are AI/ML & QIS which represented 20% of the total HEP research budget in the FY24 appropriation
- The current DOE HEP AI/ML program takes guidance from the National AI Initiative to support:
 - **Programmatic AI/ML** to address existing technical challenges using ML
 - Support for continuing efforts through base programs and all HEP NOFOs
 - **Core AI/ML** that develops new cutting-edge applications, and tools to enable broader and more advanced adoption of AI in HEP
 - New dedicated opportunities are open periodically to encourage and broaden participation
- Community planning is underway to establish near and long-term goals for the HEP AI/ML Initiative
 - These activities are expected to provide specific guidance on priorities, scope, and tools for both researchers and DOE HEP
 - Community input and engagement is welcome

Additional Material

HEP Research Breakdown (\$k) FY 2017-2024

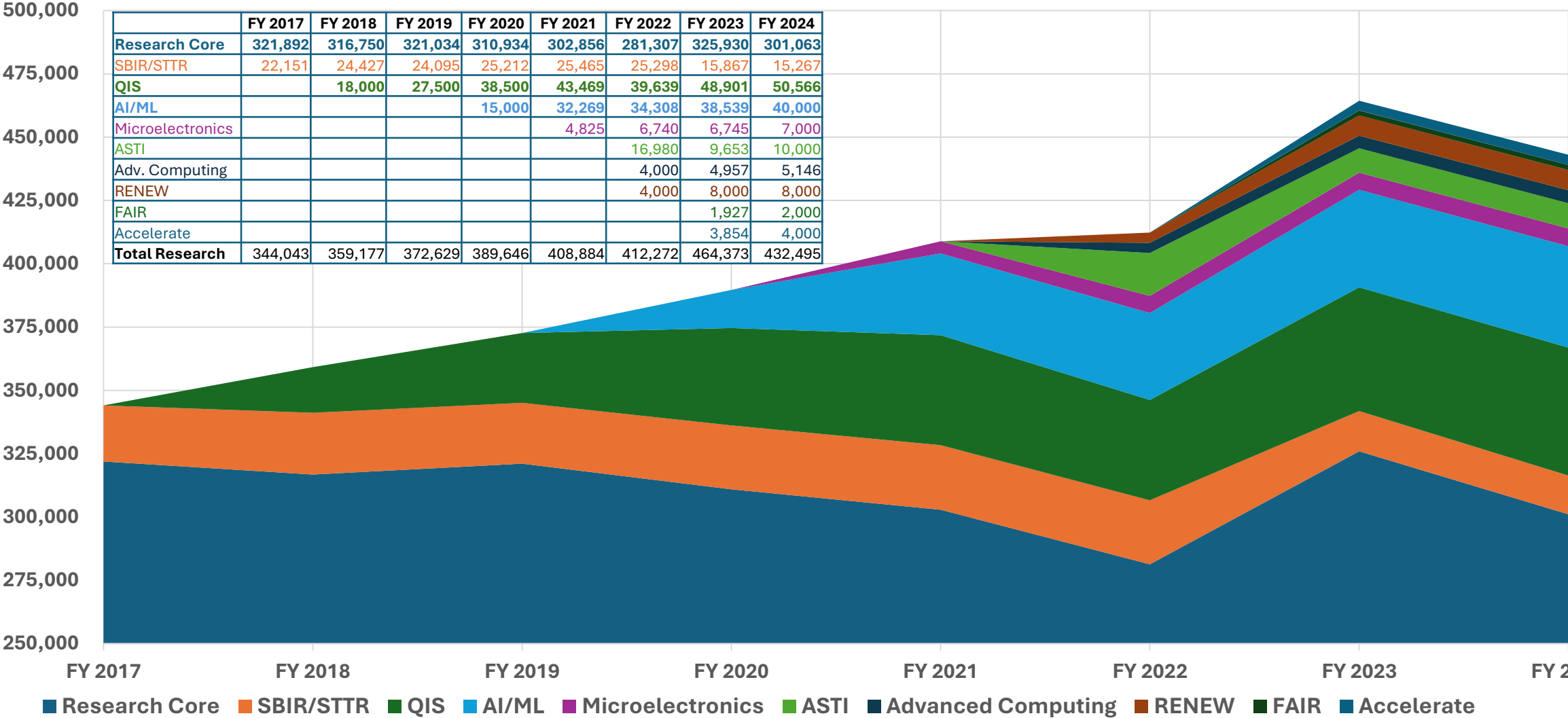


Table of AI/ML Funding by Program

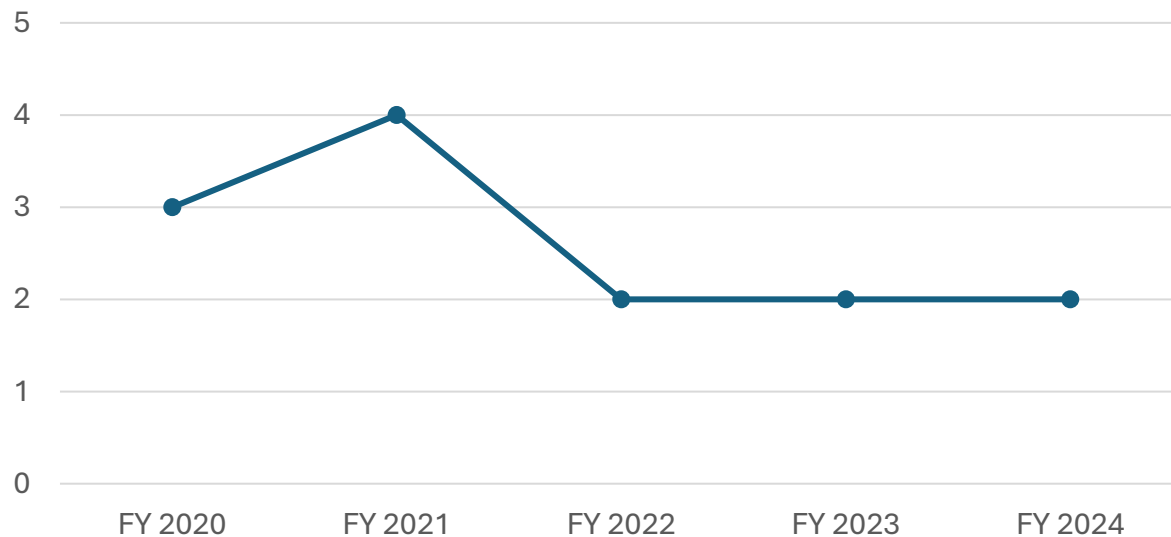
AI/ML - By Subprogram Supported

	FY 2020	FY 2021	FY 2022	FY 2023	FY 2024
Energy Frontier	4,462	10,675	9,905	8,900	5,860
Intensity Frontier	2,906	5,833	6,422	5,315	10,283
Cosmic Frontier	3,351	4,920	5,407	4,740	5,300
Theory	1,478	1,956	1,912	2,100	3,160
Comp HEP	1,350	845	3,457	11,306	2,315
GARD	1,380	7,002	6,512	4,898	4,123
Detector R&D	73	510	675	1,280	1,280

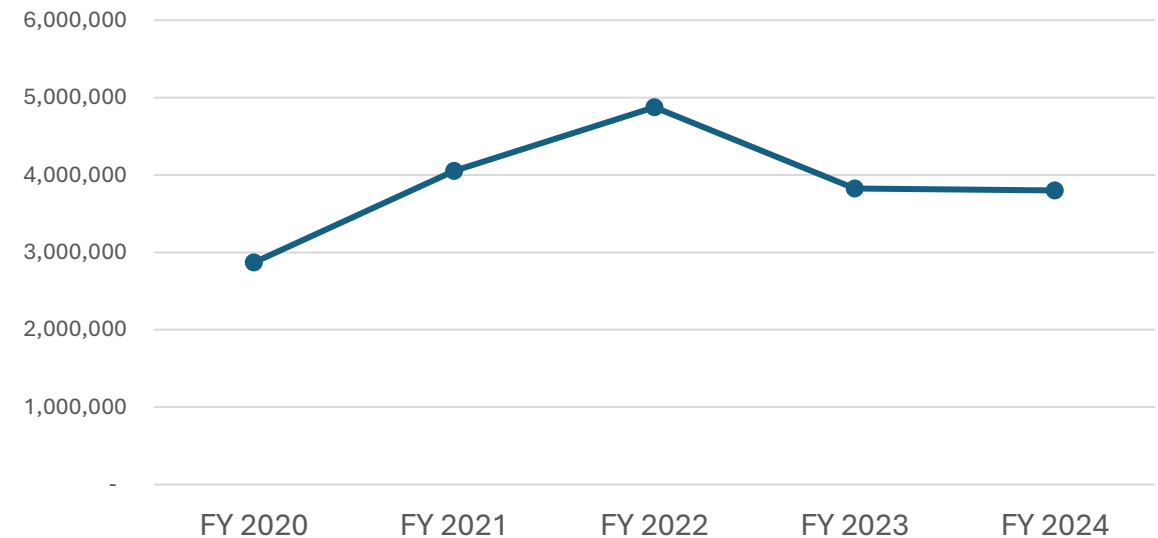
HEP AI/ML Support to the Early Career Research Program

- HEP Programmatic AI/ML has supported the Early Career Research Program since the initiative's inception
 - On average 2.6 new ECAs are supported with AI/ML funding
 - Between FY20 – FY24 \$3.9M per year of AI/ML funding supported ECAs

New AI/ML Supported Early Career Awards



Total HEP AI/ML Funding to Early Career Award



FASST: Frontiers of AI for Science, Security and Technology (aka AI for Science, Energy and Security)

Adapted from:
R. Stevens

- A large-scale DOE initiative to create world leading AI systems for accelerating science, advancing energy technologies, and improving national security
 - Led by DOE Office of Critical and Emerging Technology
- Complement AI development in industry
- Organizes, curates and prepares DOE's **vast scientific data** for training large-scale AI models \Rightarrow science foundation models
- Deploys **computing at scale** for inference, foundation model training and for AI research partnerships
- Creates **large-scale foundation models** that support DOE mission areas, supports research to advance AI fundamentals
- Develops **many AI application for improving scientific and engineering productivity** and expanding DOE capabilities
- Forms **partnerships with academia, industry and other agencies to advance AI** development and application for DOE's mission