# ARTIFICIAL INTELLIGENCE / MACHINE LEARNING FOR NUCLEAR SCIENCE

Current approaches and emerging directions

MICHELLE P. KUCHERA | DAVIDSON COLLEGE

15 April 2026 | IUPAP Nuclear Science Symposium | Rome, Italy

## AI/Machine Learning today

- Industry advances in AI
- Brief history of AI
- Brieh histor of AI in nuclear science

## Select recent work

- Automated beam tuning
- Pretrained/ Foundation Models for analysis

## Emerging community efforts/norms

- ML communities in Physics
- Physics in ML communities

## Looking forward

- Dissemination
- Ethics
- Policy
- Summary of future directions

## Machine Learning foundations

- What is Machine Learning
- A Brief History of ML
- A Brief History of ML in Nuclear Physics

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# AI Today

Widespread impact of models that generate text, **Large Language Models (LLMs),** evident in recent years.

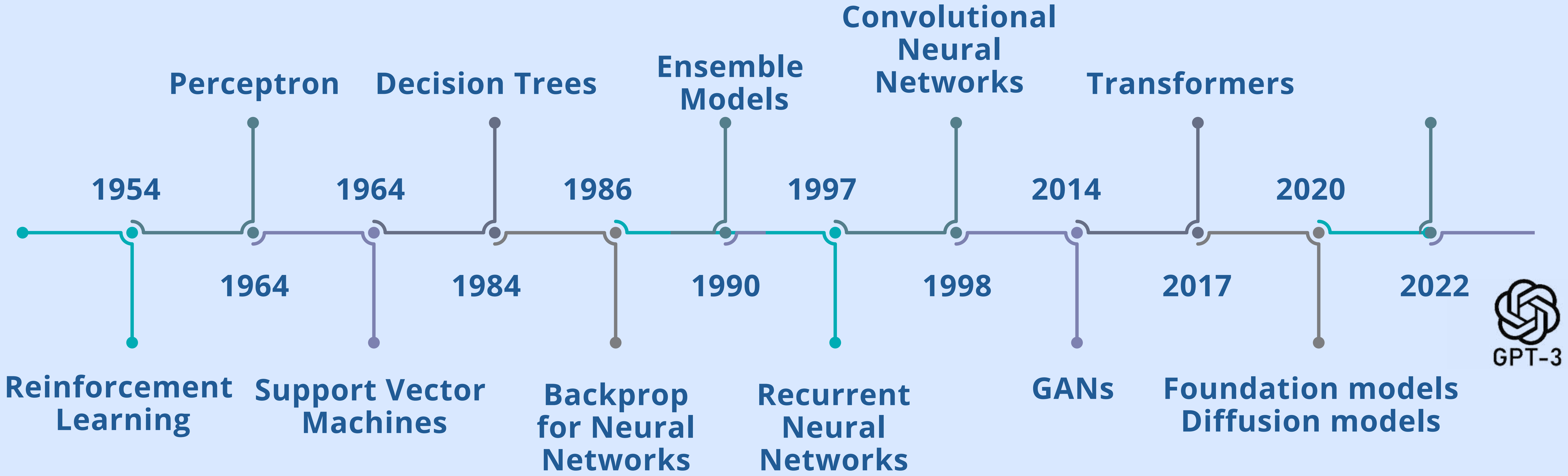
With a **user-friendly, human like interface,** we see large effects in workforce, education, daily lives, which are sparking probing discussions about benefits and drawbacks of AI in society

# AI Today

Widespread impact of models that generate text, **Large Language Models (LLMs)**, evident in recent years.

Why?

# A brief history of machine learning methods



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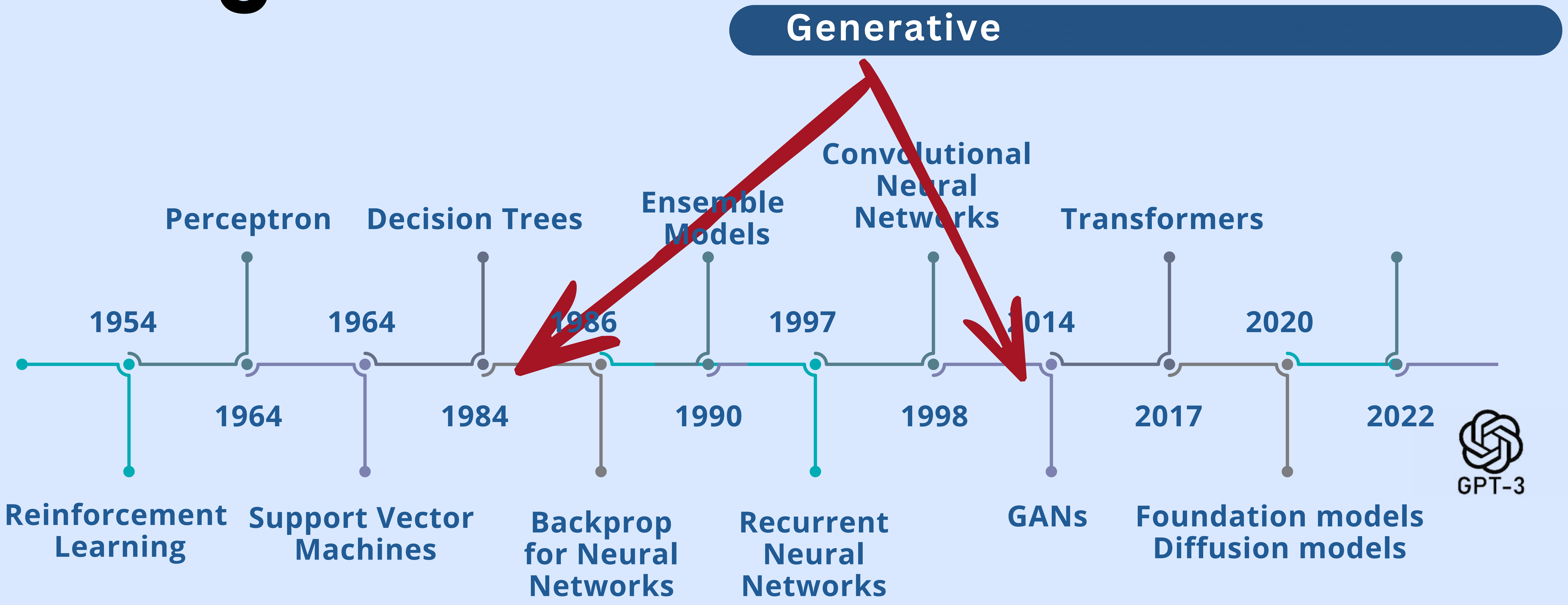

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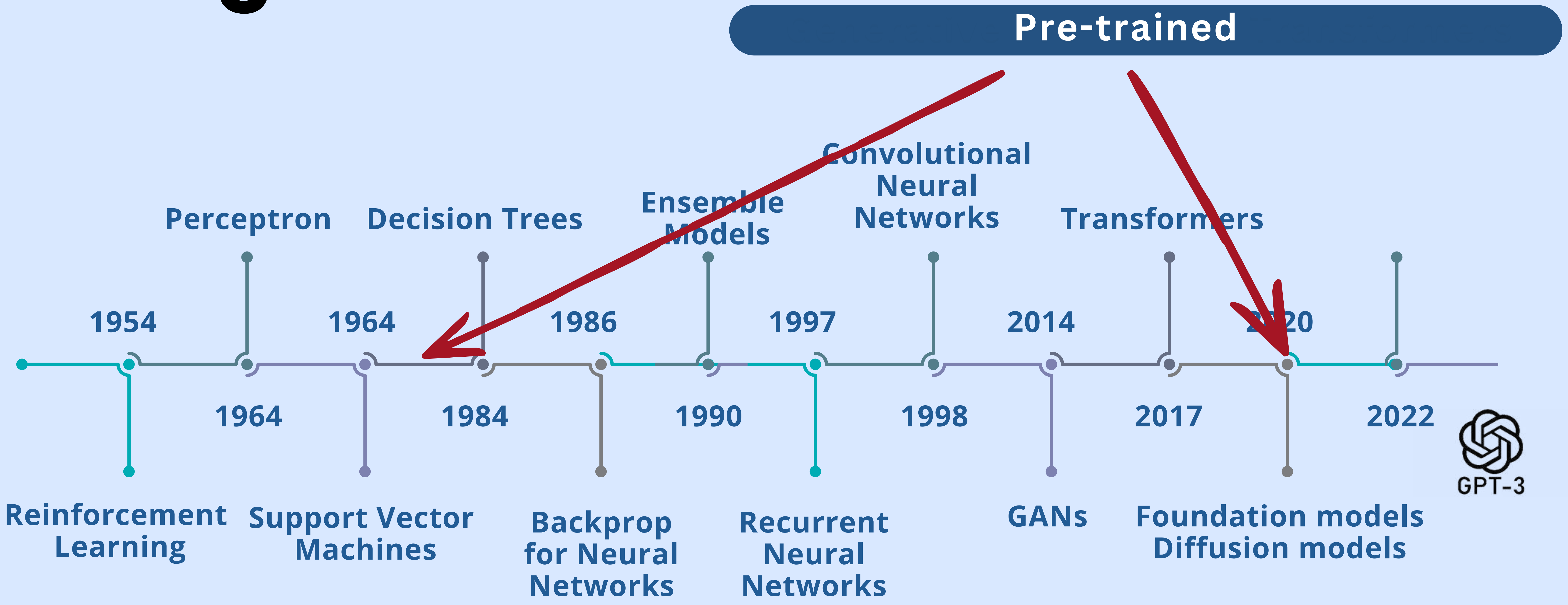

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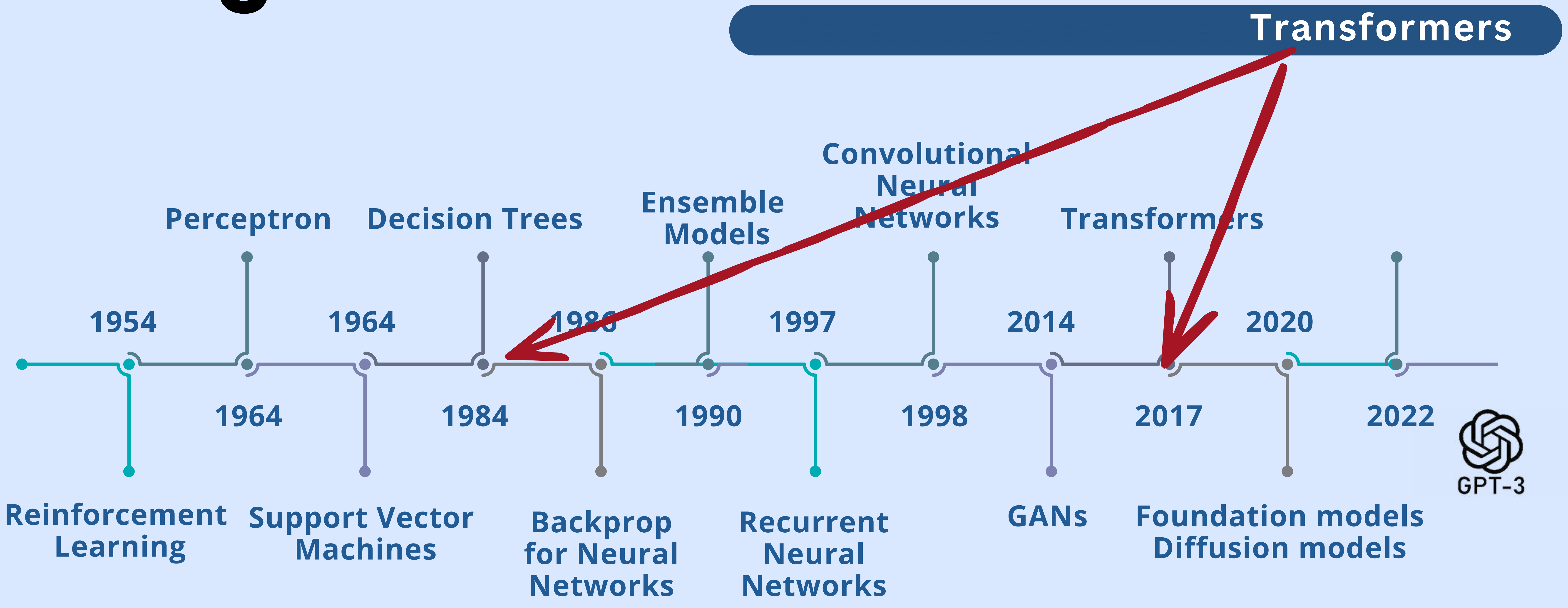

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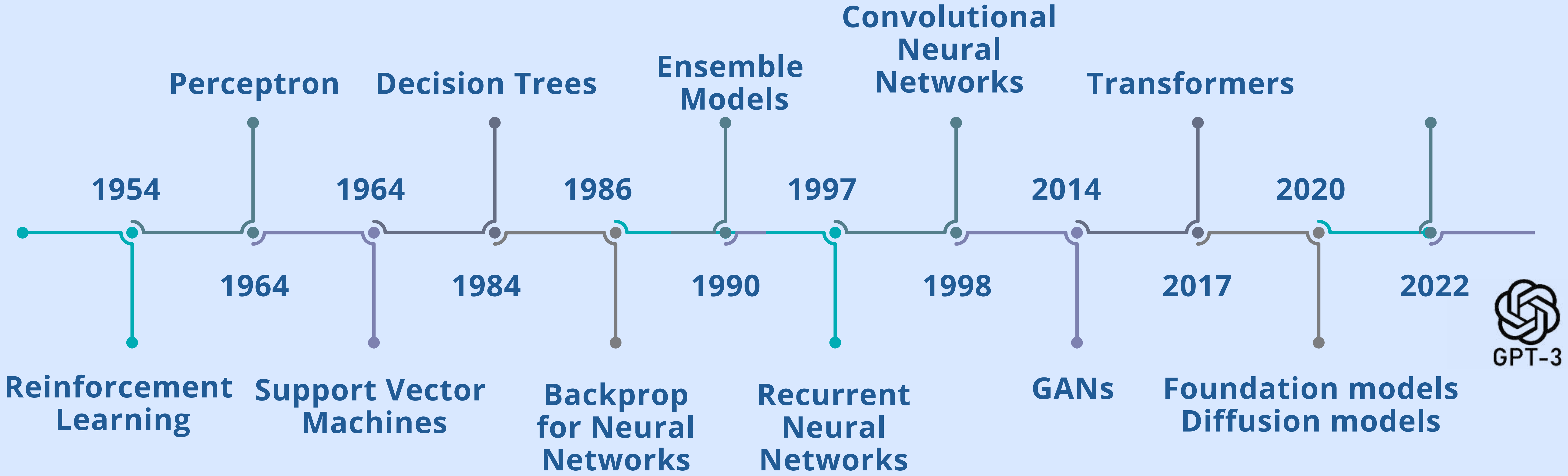
**G**enerative **P**re-trained **T**ransformers



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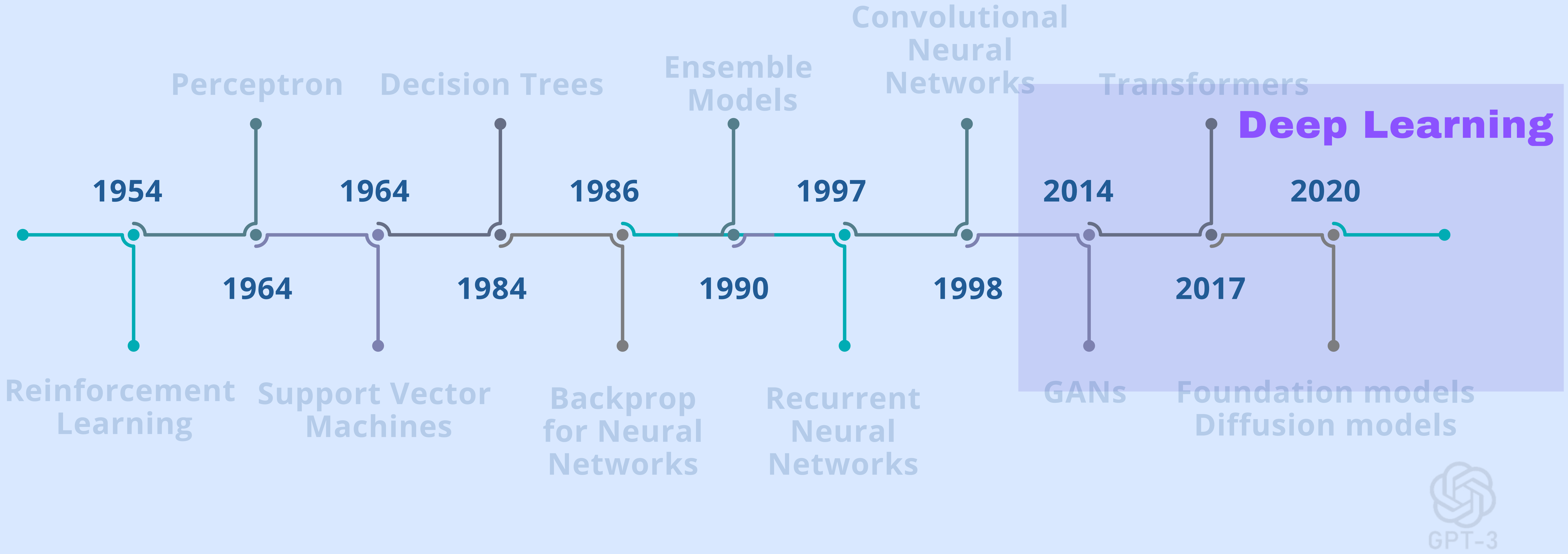

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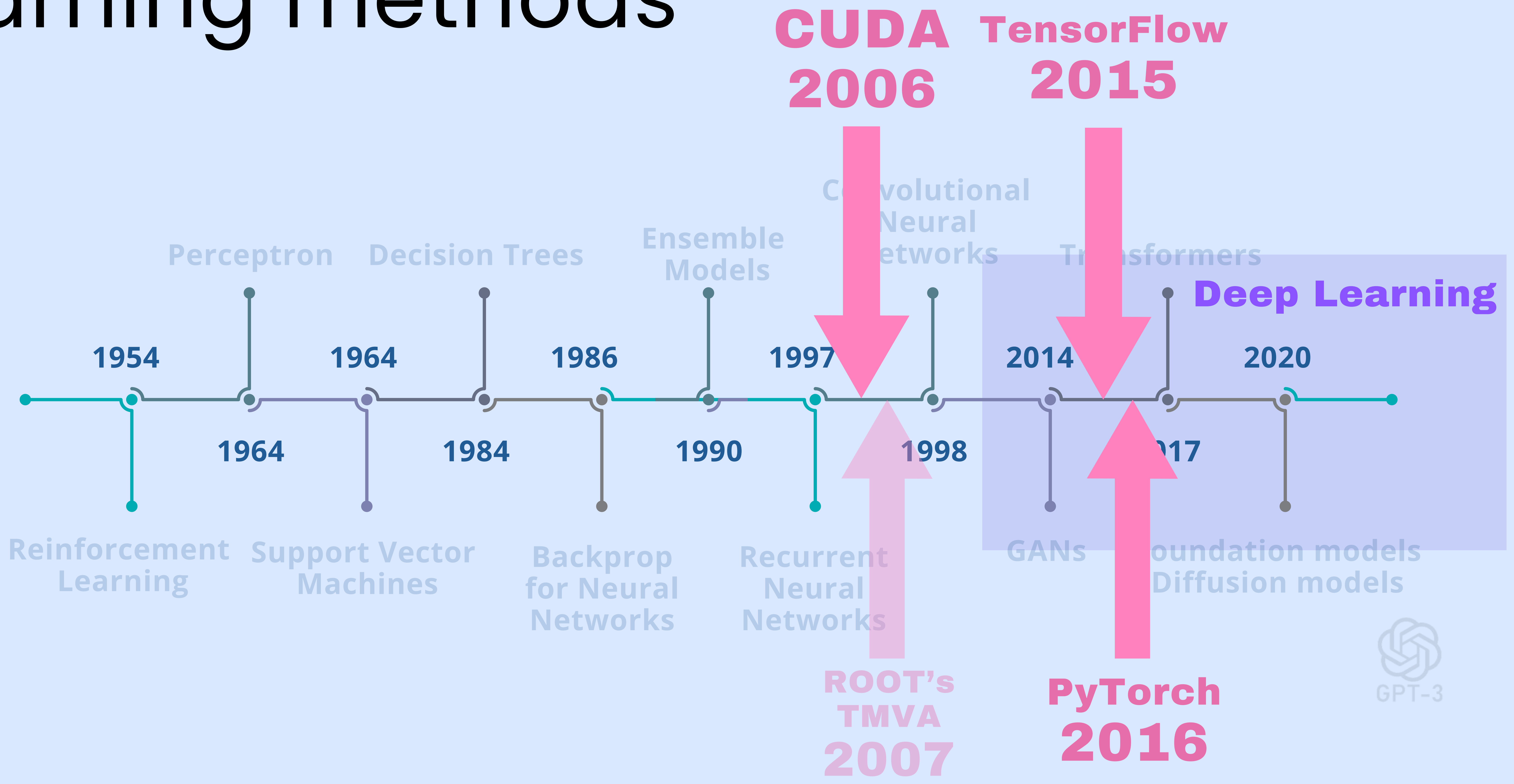

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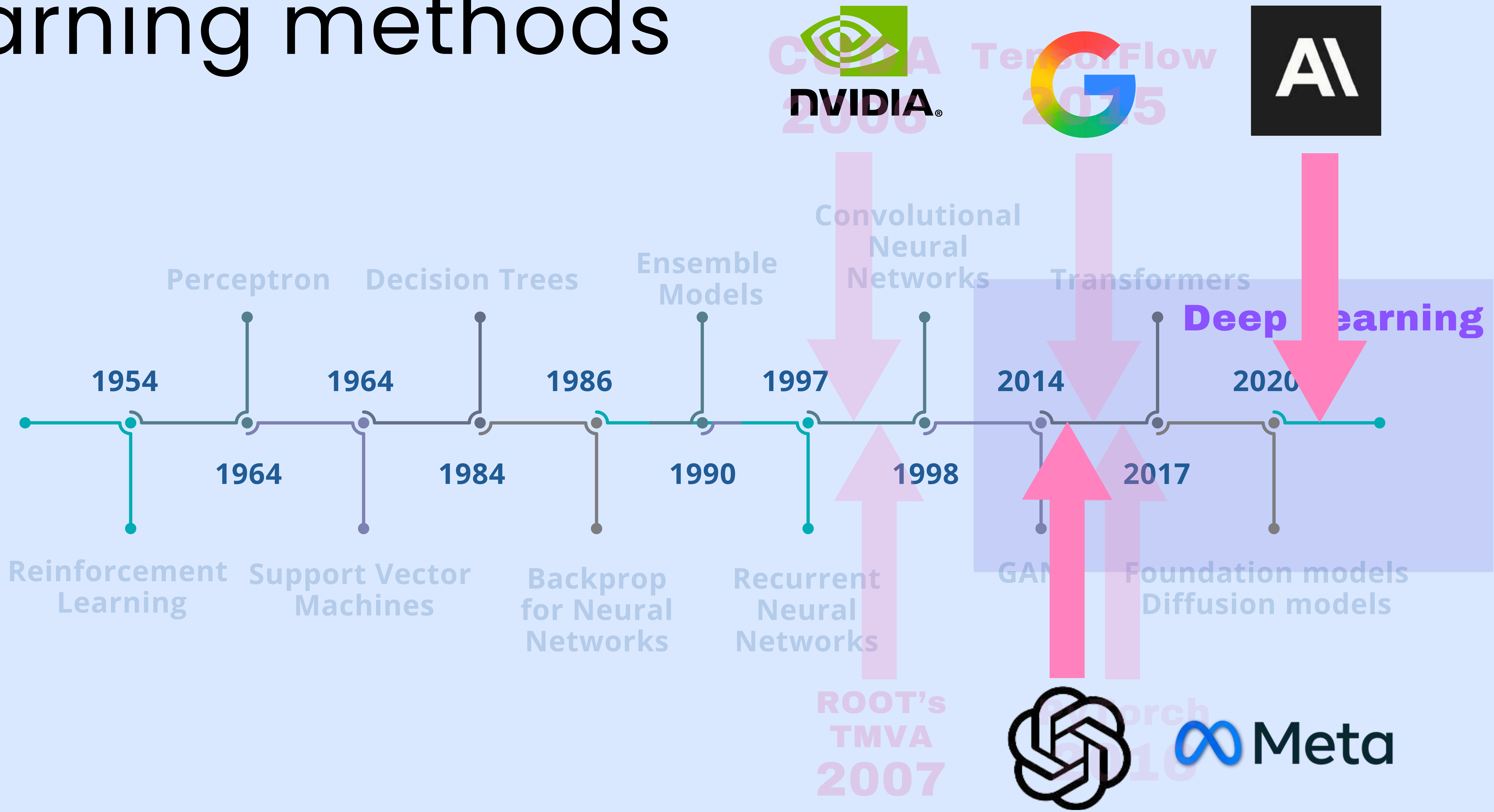


# AI Today

Widespread impact of models that generate text, **Large Language Models (LLMs),** evident in recent years.

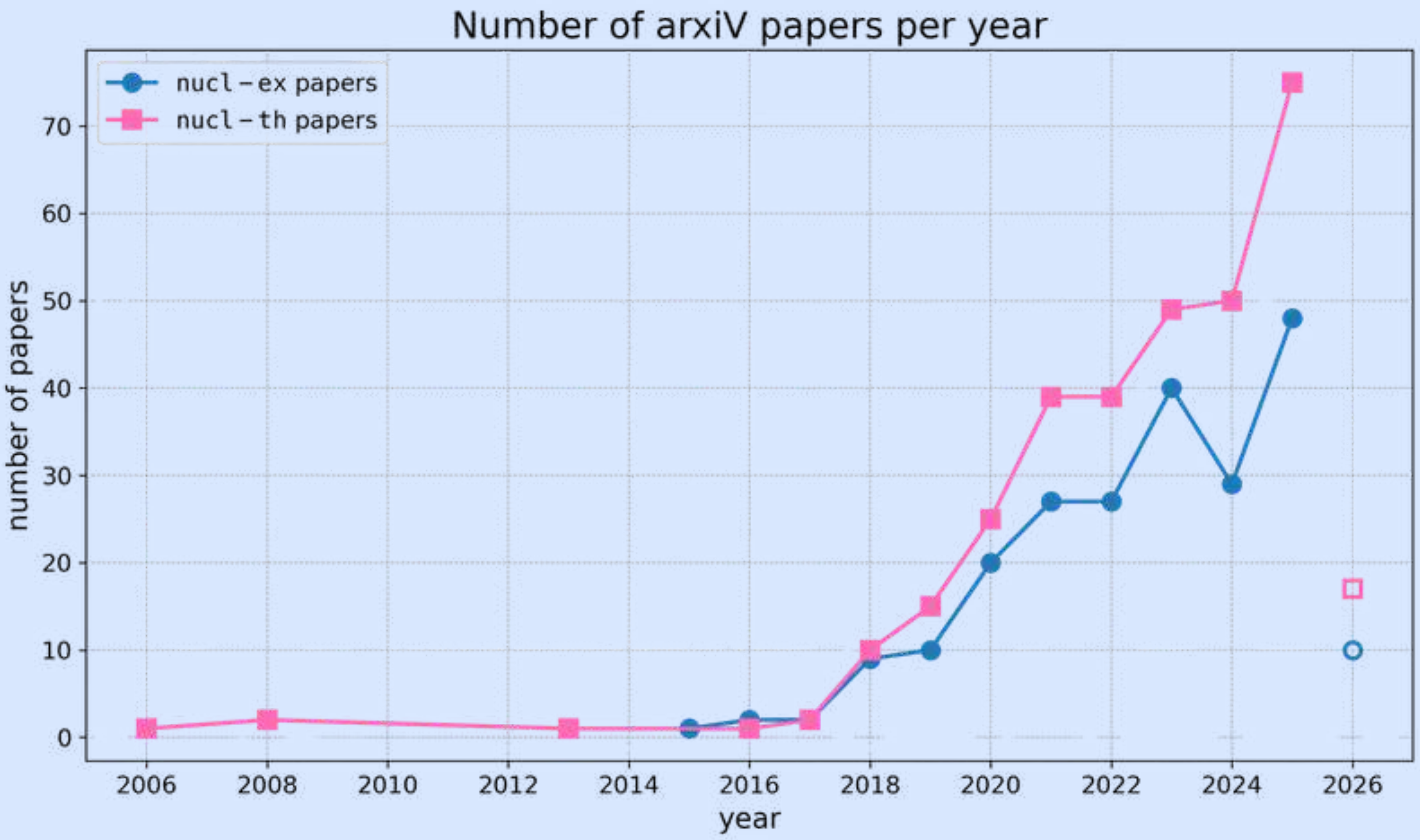
Why?

Single entity with **access to massive amounts data**

**Resources** (money, computational capacity, human power)

**User-focused interface**

# A brief history of machine learning in nuclear science




**Keywords (across all fields):**

“machine learning” OR “statistical learning” OR “deep learning”

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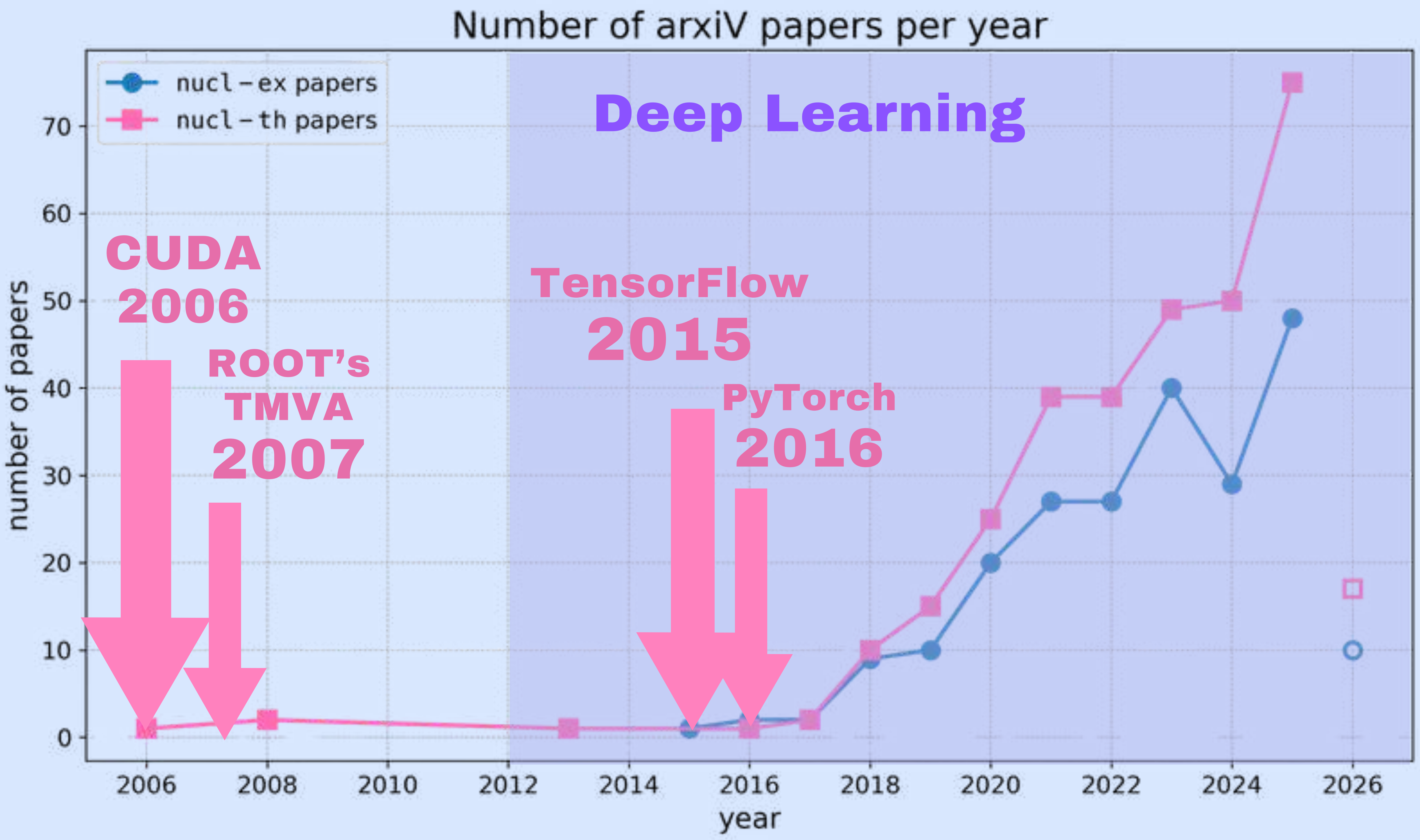


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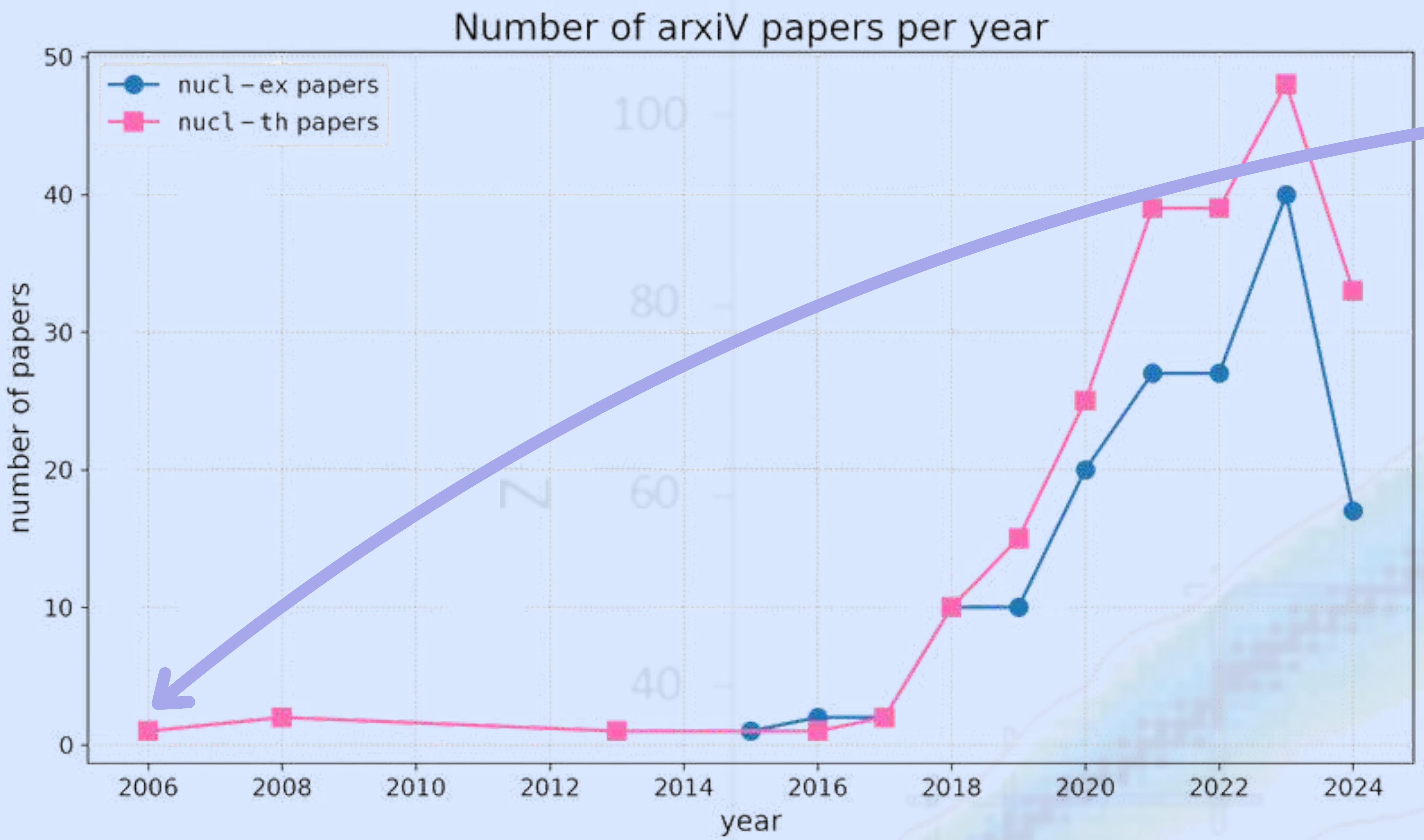


**Application Of Support Vector Machines To Global Prediction Of Nuclear Properties**
-John W Clark, Haochen Li

$(Z,N) \to M$
$(Z,N) \to T_{1/2}$

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# Recent history AI/ML in nuclear science

**Bespoke models for specific tasks/experiments/detectors**

Local progress more than global progress until very recently.

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment

Point-cloud based machine learning for classifying rare events in the Active-Target Time Projection Chamber

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment

Volume 1010, 11 September 2021, 165461

Unsupervised learning for identifying events in active target experiments

R. Solli, D. Bazin, M. Hjorth-Jensen, M.P. Kuchera, R.R. Strauss

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment

Volume 940, 1 October 2019, Pages 156-167

Machine learning methods for track classification in the AT-TPC

M.P. Kuchera, R. Ramanujan, J.Z. Taylor, R.R. Strauss, D. Bazin, J. Bradt, Ruiming Chen

Unpaired Translation of Point Clouds for Modeling Detector Response

Mingyang Li, Michelle Kuchera, Raghuram Ramanujan, Adam Anthony, Curtis Hunt, Yassid Ayyad

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment

Full Length Article

Object detection with deep learning for rare event search in the GADGET II TPC

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# Automated Beam Tuning

## Operational Accelerator Tuning via Model-Coupled Optics and Bayesian Steering

O. Hassan,[1,2] O. Shelbaya,[1,2,*] P.M. Jung,[1,2] O. Kester,[1,2] T. Planche,[1,2] and W. Fedorko[1]

[1] *TRIUMF, 4004 Wesbrook Mall, Vancouver BC, V6T 2A3, Canada*

[2] *Department of Physics and Astronomy, University of Victoria, Victoria BC, V8W 2Y2, Canada*

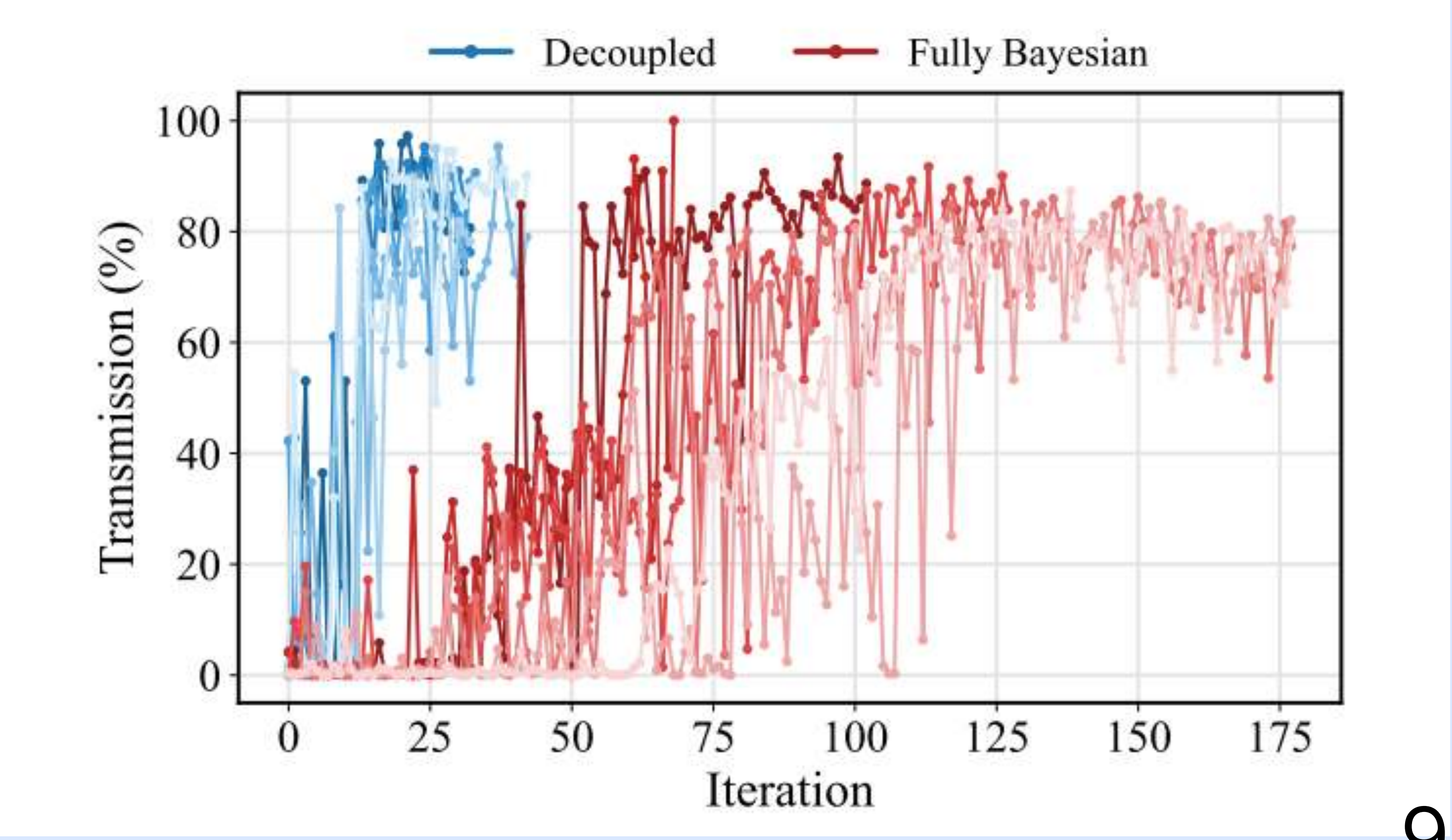
(Dated: February 25, 2026)

**Digital Twin + Bayesian Optimization @ ISAC:**

Decoupled vs Full Bayesian Approach

TABLE III. Performance of optimization strategies. Each beam was tested for both fully Bayesian and decoupled cases. Each row represents six separate optimization tests. One step corresponds to one write-measure cycle for BOIS. Conv. time requires transmission to exceed the 1% threshold to avoid noise biasing the mean, if this threshold is not reached then the conv. time is set to the maximum iteration value.

| Strategy | Species | Energy (MeV/u) | Iterations to Convergence | | Transmission (%) | |
|---|---|---|---|---|---|---|
| | | | Mean | Std. dev. | Mean | Std. dev. |
| Fully Bayesian approach | $^{16}O^{3+}$ | 0.436 | 139 | 51 | 80.3 | 25.2 |
| | $^{4}He^{+}$ | 1.60 | 174 | 6 | 4.7 | 8.8 |
| | $^{7}Li^{+}$ | 1.28 | 120 | 34 | 90.7 | 5.6 |
| Decoupled approach | $^{16}O^{3+}$ | 0.436 | 25 | 10 | 94.6 | 3.5 |
| | $^{4}He^{+}$ | 1.60 | 29 | 4 | 98.5 | 0.4 |
| | $^{7}Li^{+}$ | 1.28 | 28 | 6 | 94.7 | 2.2 |



# Foundation Models for Analysis

**TPCpp-10M: Simulated proton-proton collisions in a Time Projection Chamber for AI Foundation Models**

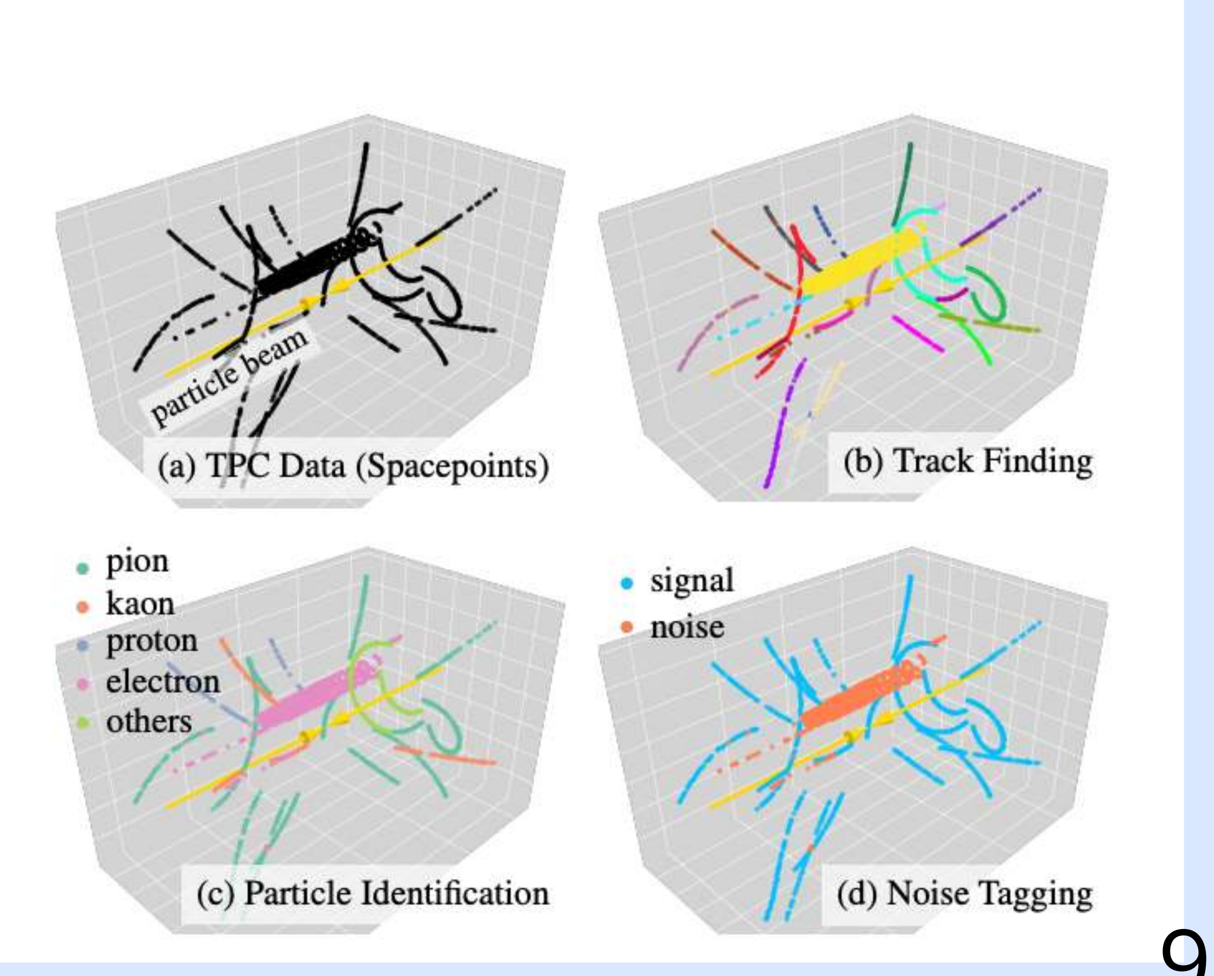
Shuhang Li[a,*], Yi Huang[b], David Park[b], Xihaier Luo[b], Haiwang Yu[c], Yeonju Go[c], Christopher Pinkenburg[c], Yuewei Lin[b], Shinjae Yoo[b], Joseph Osborn[c], Christof Roland[d], Jin Huang[c], Yihui Ren[b]

[a] *Department of Physics, Columbia University, New York, NY, USA*
[b] *AI Department, Brookhaven National Laboratory, Upton, NY, USA*
[c] *Nuclear and Particle Physics Department, Brookhaven National Laboratory, Upton, NY, USA*
[d] *Department of Physics, Massachusetts Institute of Technology, Cambridge, MA, USA*

**FM4NPP: A Scaling Foundation Model for Nuclear and Particle Physics**

**David Park[*1], Shuhang Li[*2], Yi Huang[*1], Xihaier Luo[1], Haiwang Yu[2], Yeonju Go[2], Christopher Pinkenburg[2], Yuewei Lin[1], Shinjae Yoo[1], Joseph Osborn[2], Jin Huang[2], Yihui Ren[1]**

[1] AI Department, Brookhaven National Laboratory, Upton, NY
[2] Nuclear and Particle Physics Department, Brookhaven National Laboratory, Upton, NY
{dpark1, sli7, yhuang2, xluo, hyu, ygo, pinkenbu, ywlin, sjyoo, josborn1, jhuang, yren}@bnl.gov

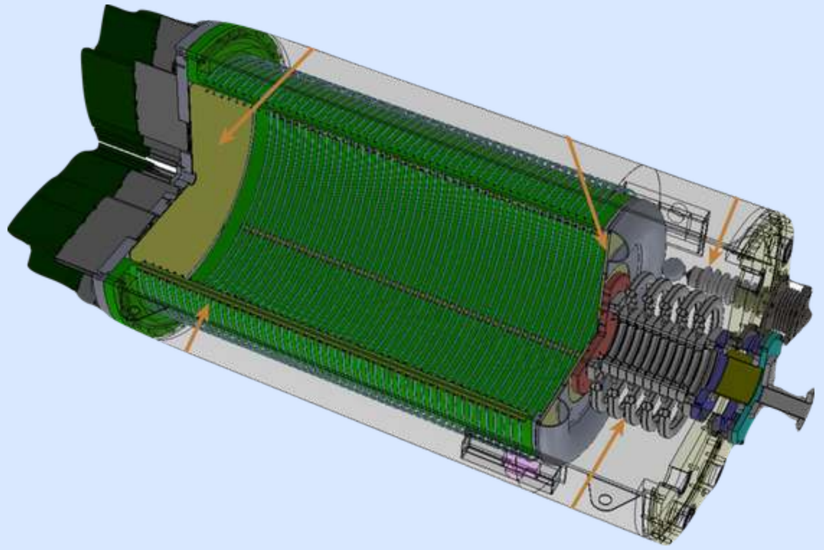


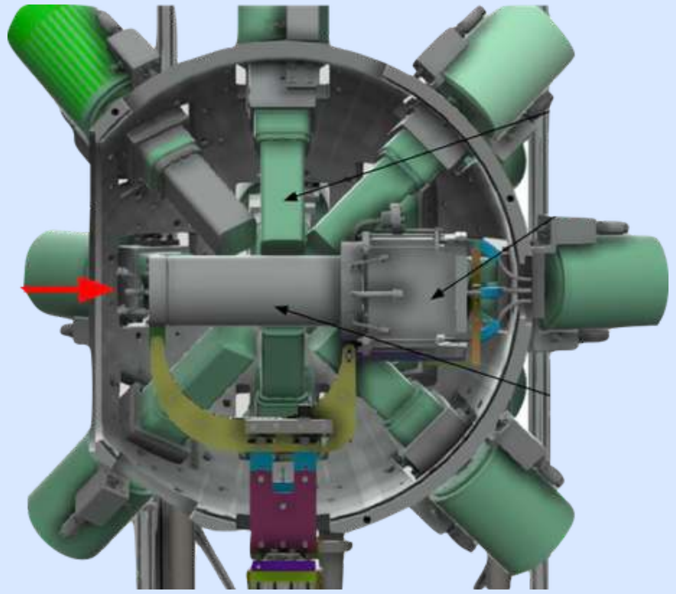

**Digital Twin + Bayesian Optimization @ ISAC:**
Decoupled vs Full Bayesian Approach

# Foundation Models for Analysis

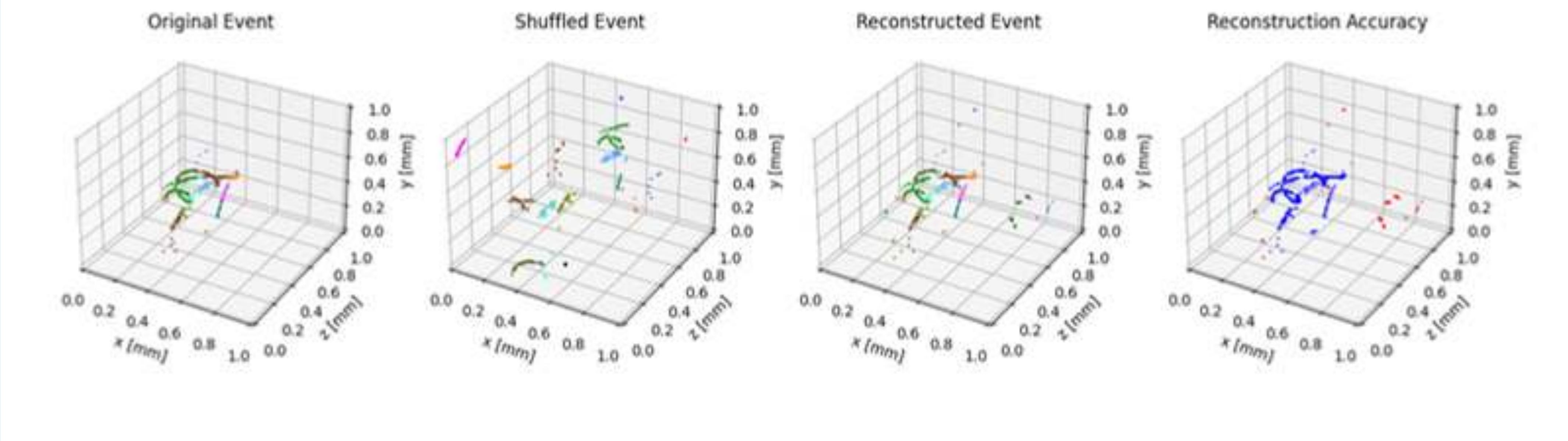
## Sparse Methods for Vector Embeddings of TPC Data

Tyler Wheeler[1] Michelle P. Kuchera[2] Raghuram Ramanujan[2]
Ryan Krupp[1] Chris Wrede[1] Saiprasad Ravishankar[1]
Connor L. Cross[2] Hoi Yan Ian Heung[2] Andrew J. Jones[2] Benjamin Votaw[2]
[1] Michigan State University [2] Davidson College
wheele56@msu.edu {mikuchera,raramanujan}@davidson.edu
{krupprya,wrede,ravisha3}@msu.edu
{cocross,iaheung,anjones1,bevotaw}@davidson.edu





| Domain | Accuracy | | | F1 Score | | |
|---|---|---|---|---|---|---|
| | $\texttt{ResNet}_{train}$ | $\texttt{ResNet}_{rand}$ | Naïve | $\texttt{ResNet}_{train}$ | $\texttt{ResNet}_{rand}$ | Naïve |
| GADGET II | **0.97** | 0.85 | 0.33 | **0.97** | 0.85 | 0.17 |
| AT-TPC | **0.74** | 0.58 | 0.48 | **0.70** | 0.53 | 0.31 |



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# Roadmap for ML in Nuclear Science

## 2020 AI for Nuclear Physics workshop
## Community Identified Needs and Commonalities:

- Workforce development
  - educational activities
  - community: centralized, value interdisciplinary work
  - collaboration with ML community

Jefferson Lab

Group photo from the workshop AI for Nuclear Physics held at Thomas Jefferson National Accelerator Facility on March 4-6, 2020.

## 2020 AI for Nuclear Physics workshop Community Identified Needs and Commonalities:

- Workforce development
  - educational activities
  - community: centralized, value interdisciplinary work
  - collaboration with ML community
- Uncertainty quantification
- appropriate use of industry-standard tools
- problem-specific tools
- comprehensive data management
- adequate computational resources

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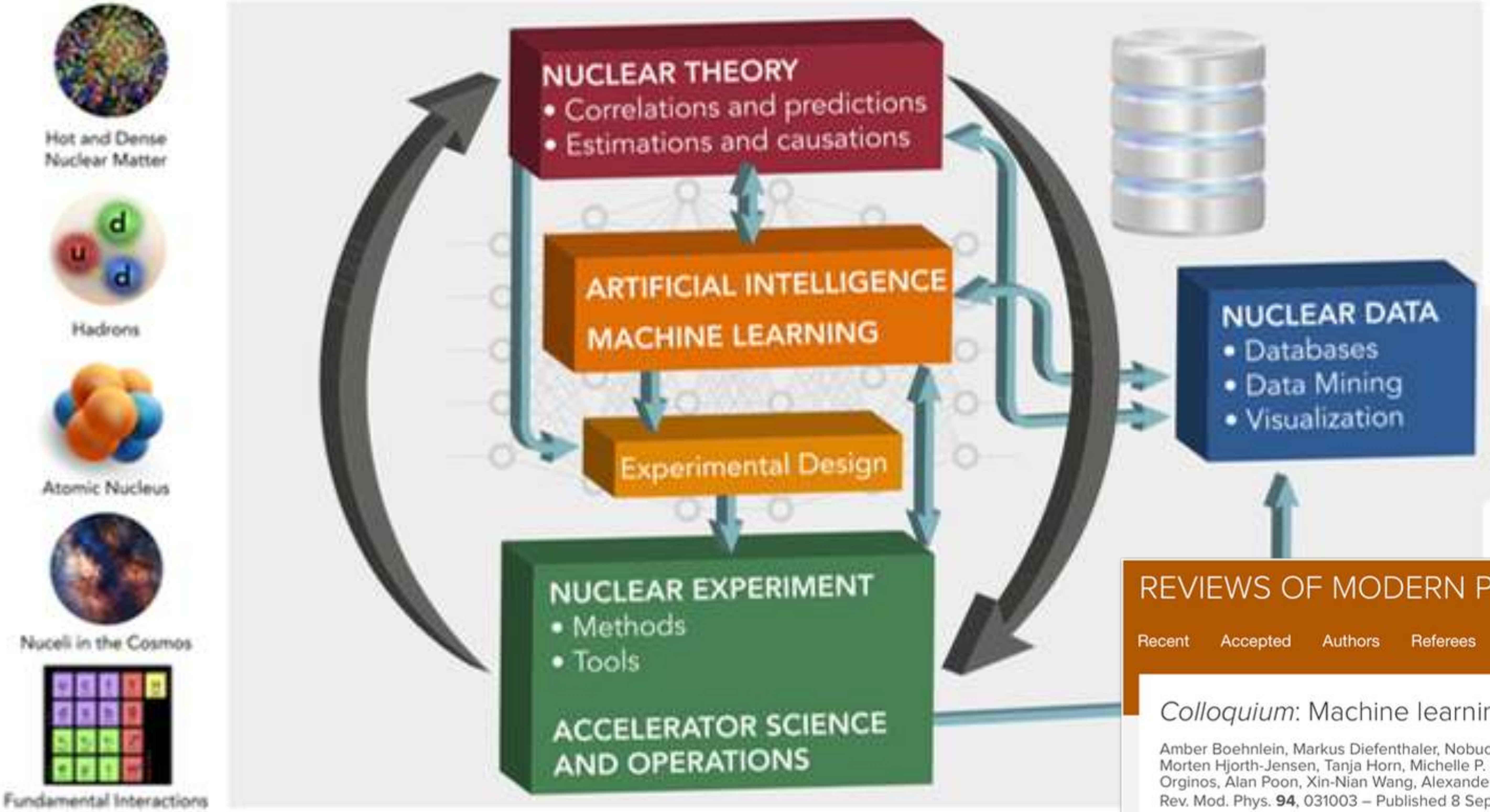
# A brief history of machine learning in nuclear science

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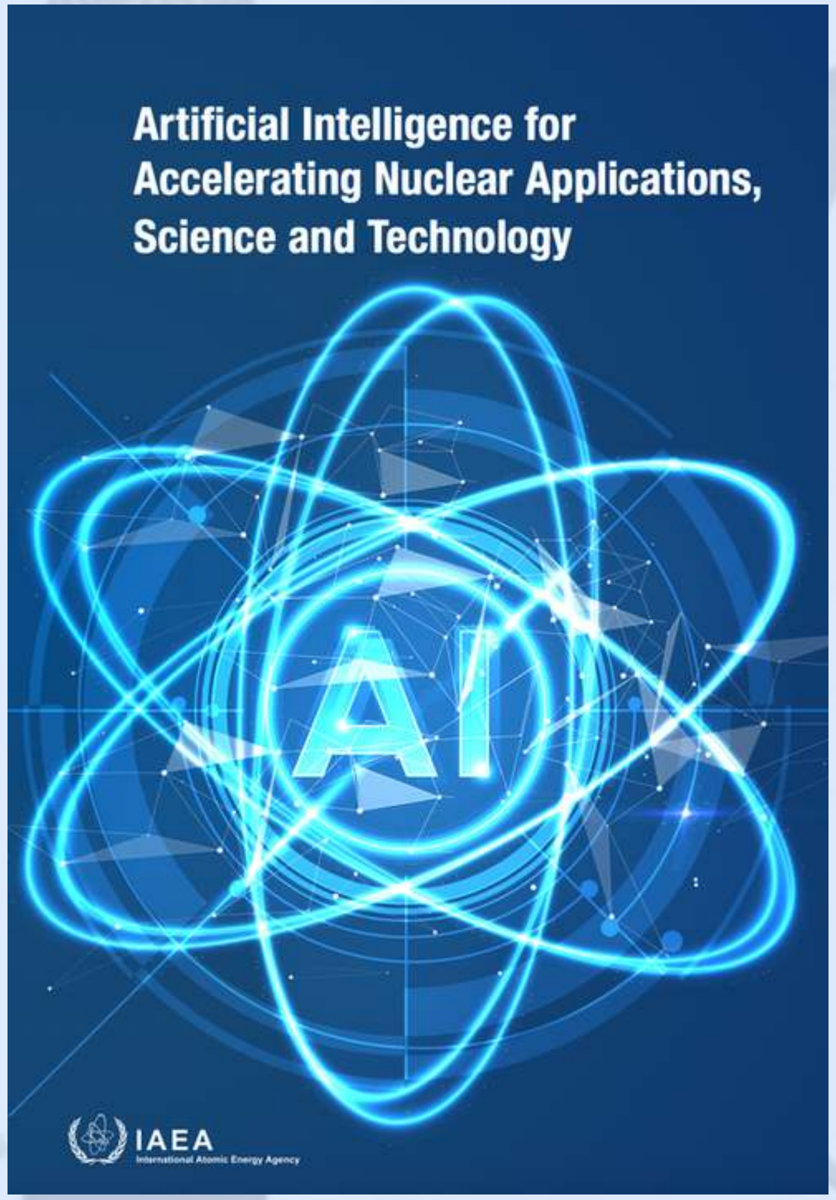
*Colloquium*: Machine learning in nuclear physics

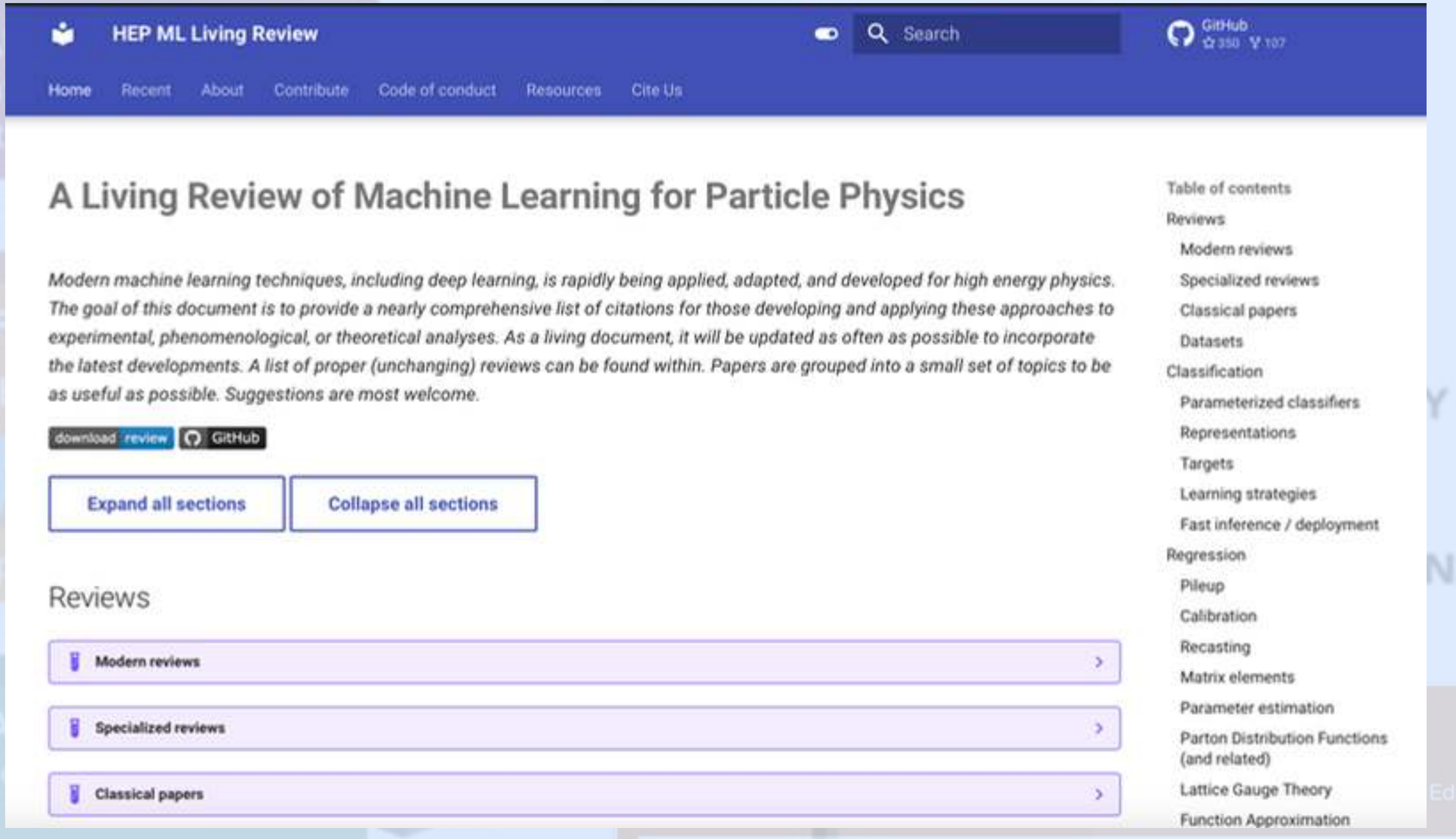
Amber Boehnlein, Markus Diefenthaler, Nobuo Sato, Malachi Schram, Veronique Ziegler, Cristiano Fanelli, Morten Hjorth-Jensen, Tanja Horn, Michelle P. Kuchera, Dean Lee, Witold Nazarewicz, Peter Ostroumov, Kostas Orginos, Alan Poon, Xin-Nian Wang, Alexander Scheinker, Michael S. Smith, and Long-Gang Pang

Rev. Mod. Phys. **94**, 031003 – Published 8 September 2022

# A brief history of machine learning in nuclear science




**2022**

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Rev. Mod. Phys. 94, 031003 – Published 8 September 2022 management within an emerging heterogeneous infrastructure of resources that connects facilities and academic institutions to decentralized storage architectures and federated and industrial computing clusters. Delivering developer productivity and performance portability in this web of computing resources will require composing nuclear workflows from existing workloads and data deployed across multiple organizations.

### 10.4 ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING

The ongoing revolution in the field of AI/ML has significantly influenced the nuclear physics community. For example, EIC could be one of the first large-scale collider-based programs in which AI/ML is integrated from the start. This development is hardly surprising because the nuclear physics community has been an early adopter of other innovative computer technologies and has frequently led their development. ML techniques are already standard in several branches of experimental and theoretical nuclear physics. Recent developments include the following:

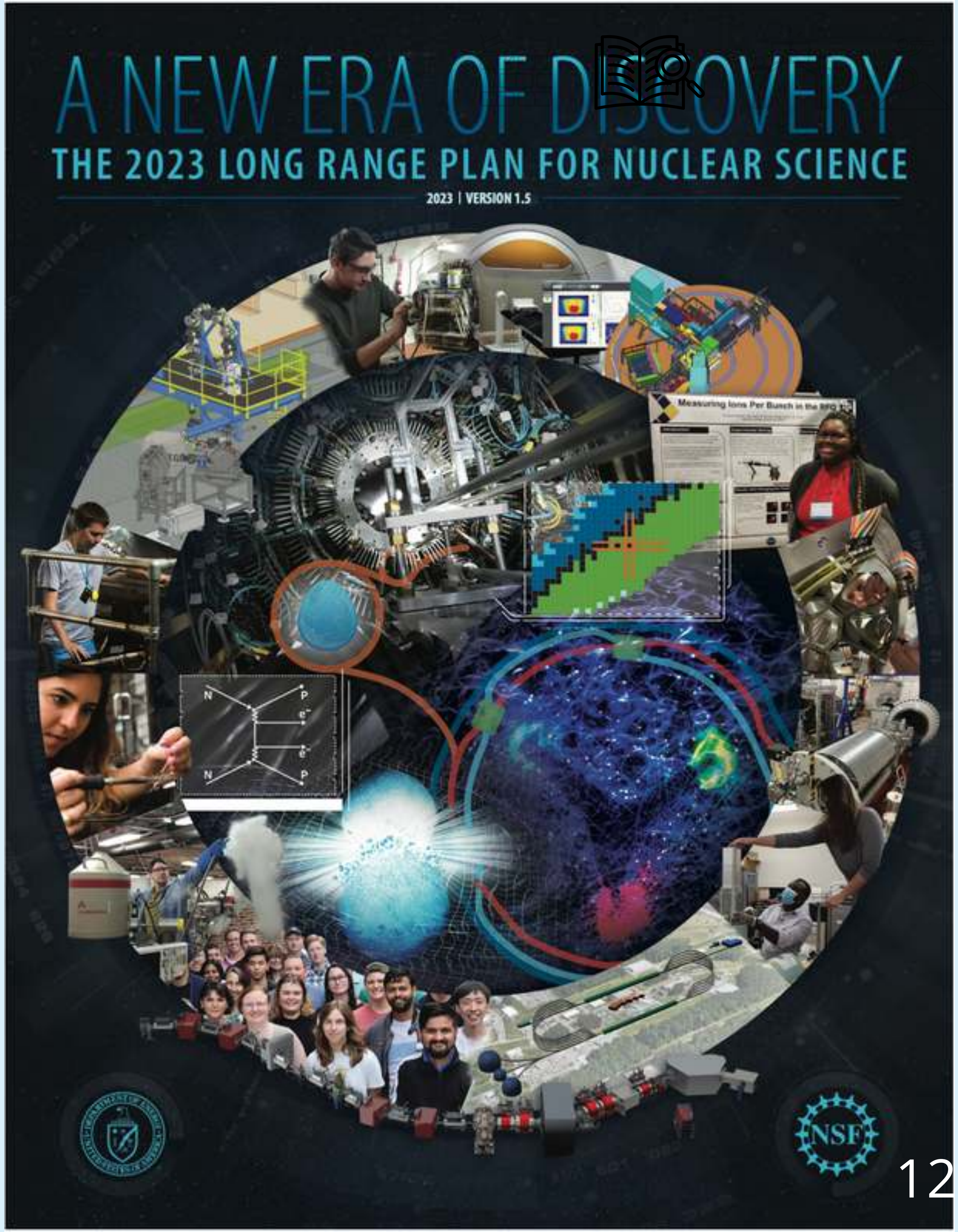
- Automation and/or optimization of the operation of accelerators and detector systems, including development and validation of virtual diagnostics, improvement to beam sources and injector performance, data-driven system maintenance, automated learning for operator support, and anomaly detection and mitigation.
- Improved Monte Carlo calculations for lattice QCD and new approaches to solve the Monte Carlo sign-problem by ML-assisted contour deformation. These examples demonstrate AI/ML accelerating progress in nuclear theory.
- Systematic improvement of variational nuclear wave functions. The simple wave functions used in variational Monte Carlo, which are based on insight gained throughout many decades, are now being substituted with parametrizations using neural networks and their automatic optimization. These techniques have the promise to automate the process of discovery.
- Improved experimental design and real-time tuning, including improving experiments by intelligently combining disparate data sources such as accelerator parameters, experimental controls, and detector data. AI/ML enables intelligent decisions about data reduction and storage and can improve the physics content by using data compression, sophisticated triggers (both software- and hardware-based), continuous data quality control and calibration, task-based high-performance local computing, distributed bulk data processing at supercomputer centers, and online analytical processing.
- Improving simulation and analysis, including (1) improving sensitivity to allow more information to be extracted from datasets, decreasing uncertainty in results and increasing discovery potential; (2) decreasing simulation and analysis time to save costs and allow for a higher volume of scientific output by accelerating the feedback loop between experiment, analysis, and theory.

These developments highlight the significant amount of recent exploratory research and suggest a near-term increase by orders of magnitude in the use of AI/ML methods. Nuclear physics offers rich, complex data sets, ideally suited for AI/ML methods. It also provides rigorous, well-controlled contexts in which AI/ML successes and failures can be clearly distinguished. It is an ideal place to explore issues of interpretability and/or alignment that are much more difficult to approach in less contained datasets and pursued less vigorously by private enterprise.

The rapid growth in the field also poses some challenges to the field of nuclear physics. One of the lessons learned in the last decade is that AI/ML techniques become useful only at scale, when computational resources are substantial. Reaching this scale poses a challenge for individual researchers, especially those not connected to collaborations and/or experiments with significant computer resources. Furthermore, the application of AI/ML methods to different aspects of nuclear research is a high-payoff, low-yield enterprise. As such, we require a funding model that can provide timely resources, is not risk adverse, and embraces innovation. Mechanisms to foster communication between researchers within the nuclear physics and AI/ML communities should also be developed. Retention should be an important part of any AI/ML strategy for nuclear physics, because private-sector opportunities create a challenge to keep people with AI/ML expertise in nuclear physics.

### 10.5 QUANTUM INFORMATION, QUANTUM COMPUTING, AND QUANTUM SENSING

DOE, NSF, NIST, and other funding agencies are substantially investing in basic research for QIST and its applications. This investment has greatly benefited research at the interface of nuclear physics and QIST, has yielded important advances and benchmarking for future research, and is growing interdisciplinary collaborations.



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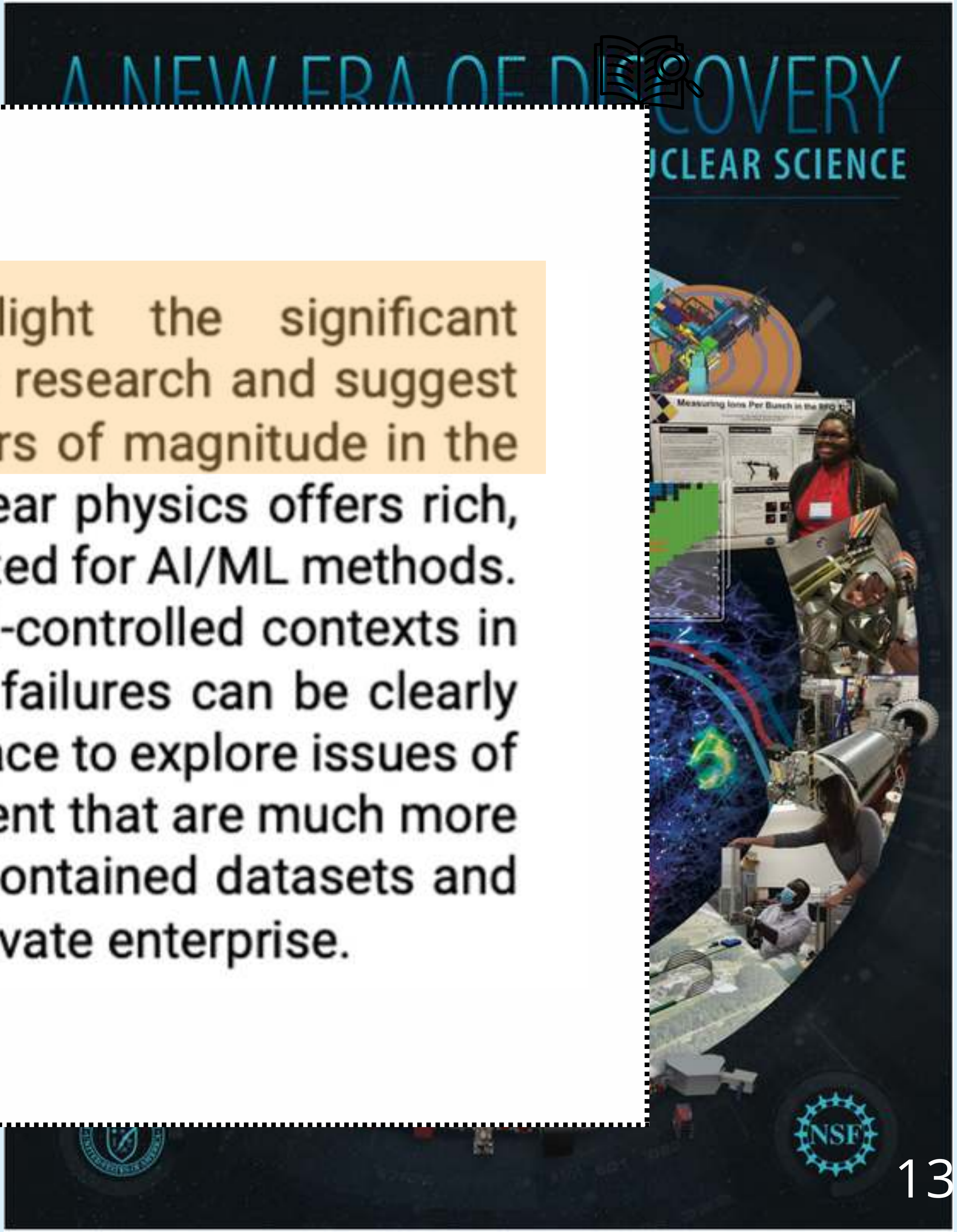

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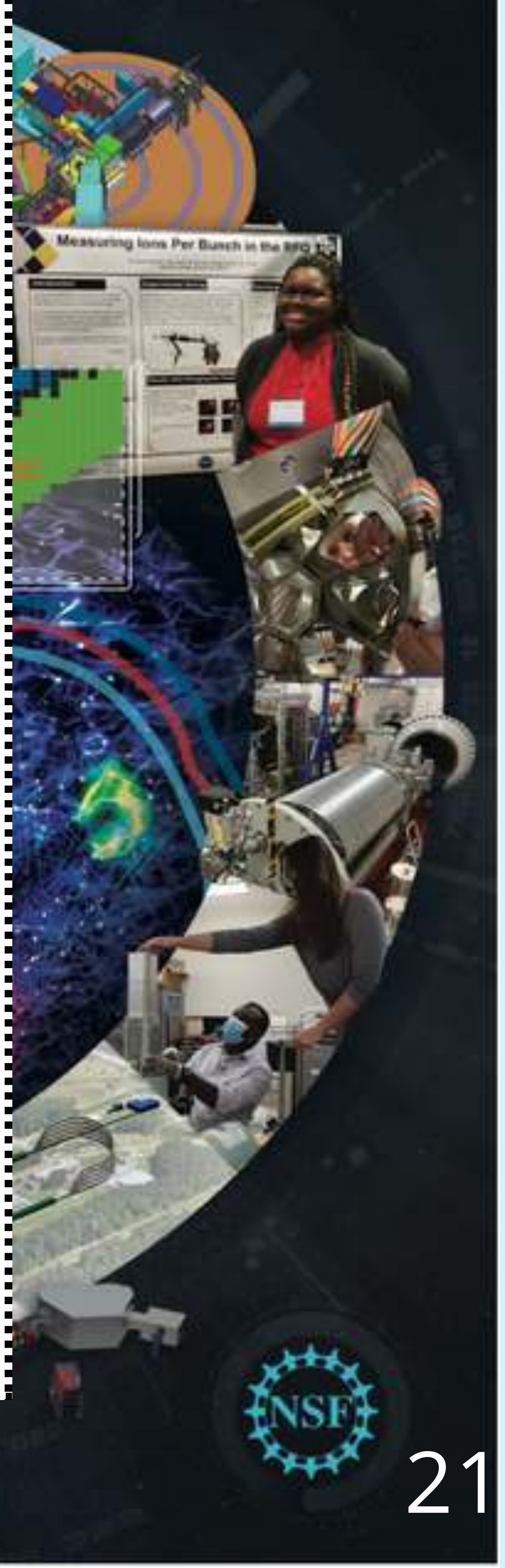


# Emerging Communities

EuCAIF

Genesis Mission

The NSF Institute for
Artificial Intelligence and
Fundamental Interactions

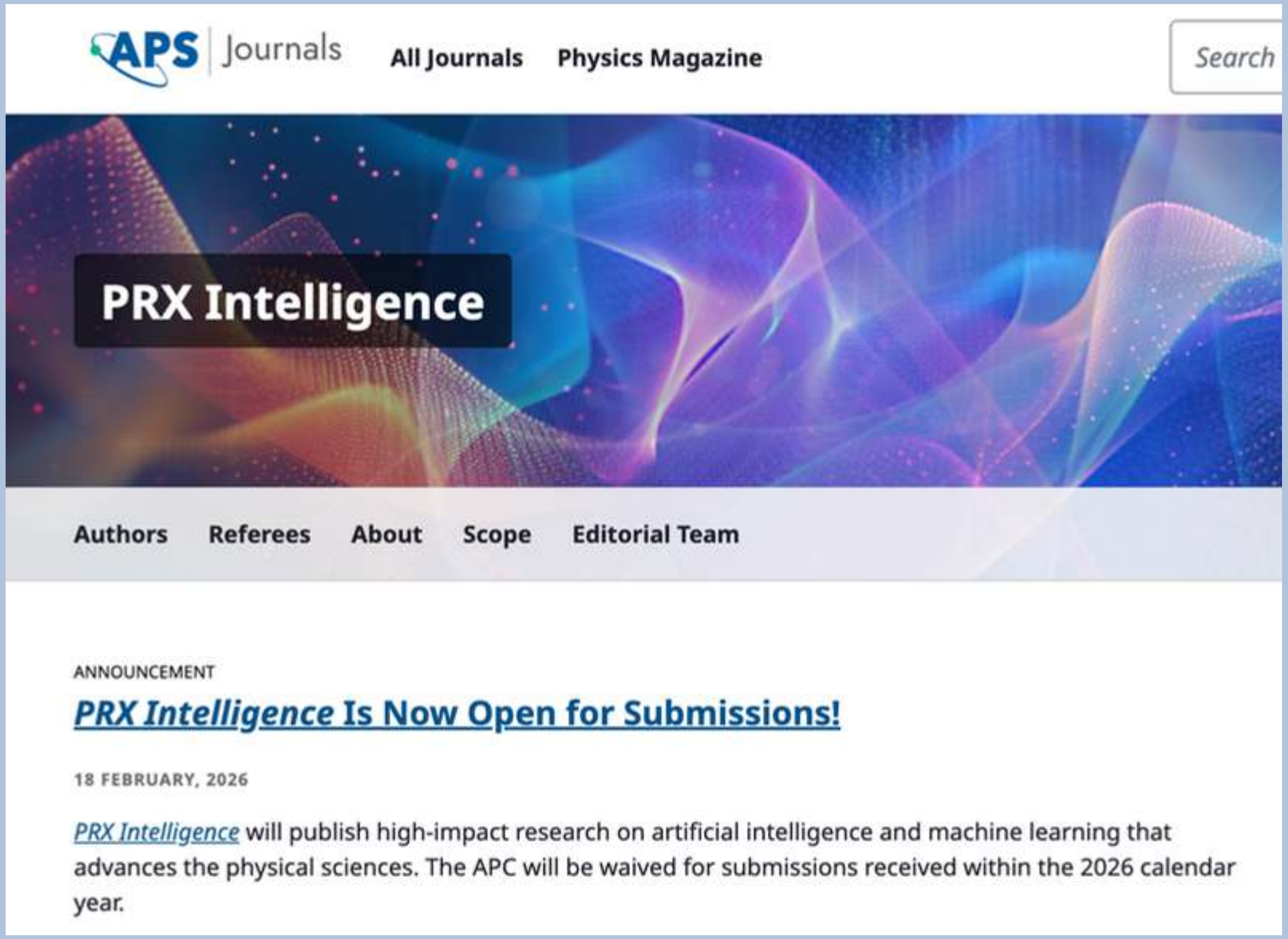
Machine Learning Applications for
Particle Accelerators

hls 4 ml

BAND
Bayesian Analysis of Nuclear Dynamics

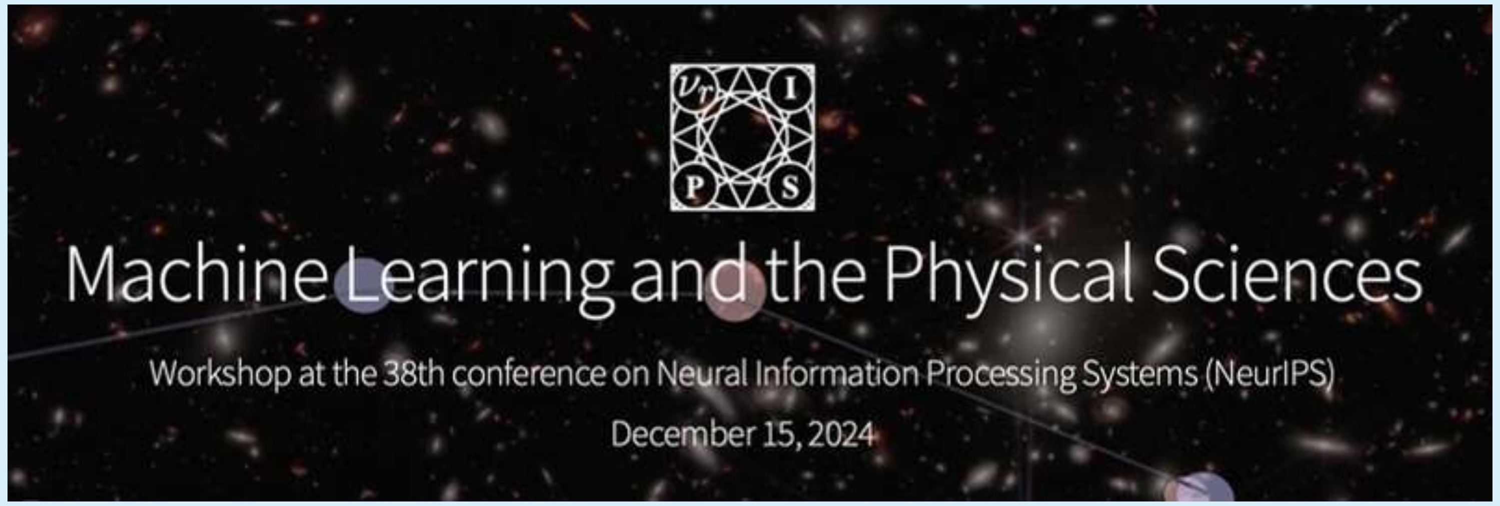
AI4EIC

# Emerging Communities




# Emerging Communities

NEURAL INFORMATION
PROCESSING SYSTEMS




**2016-2026: Machine Learning and the Physical Sciences**

ICML
International Conference
On Machine Learning

**2023: Physics for ML**
**2024: <u>AI for Science: Scaling in AI for Scientific Discovery</u>**
**<u>2026: AI for Physics</u>**

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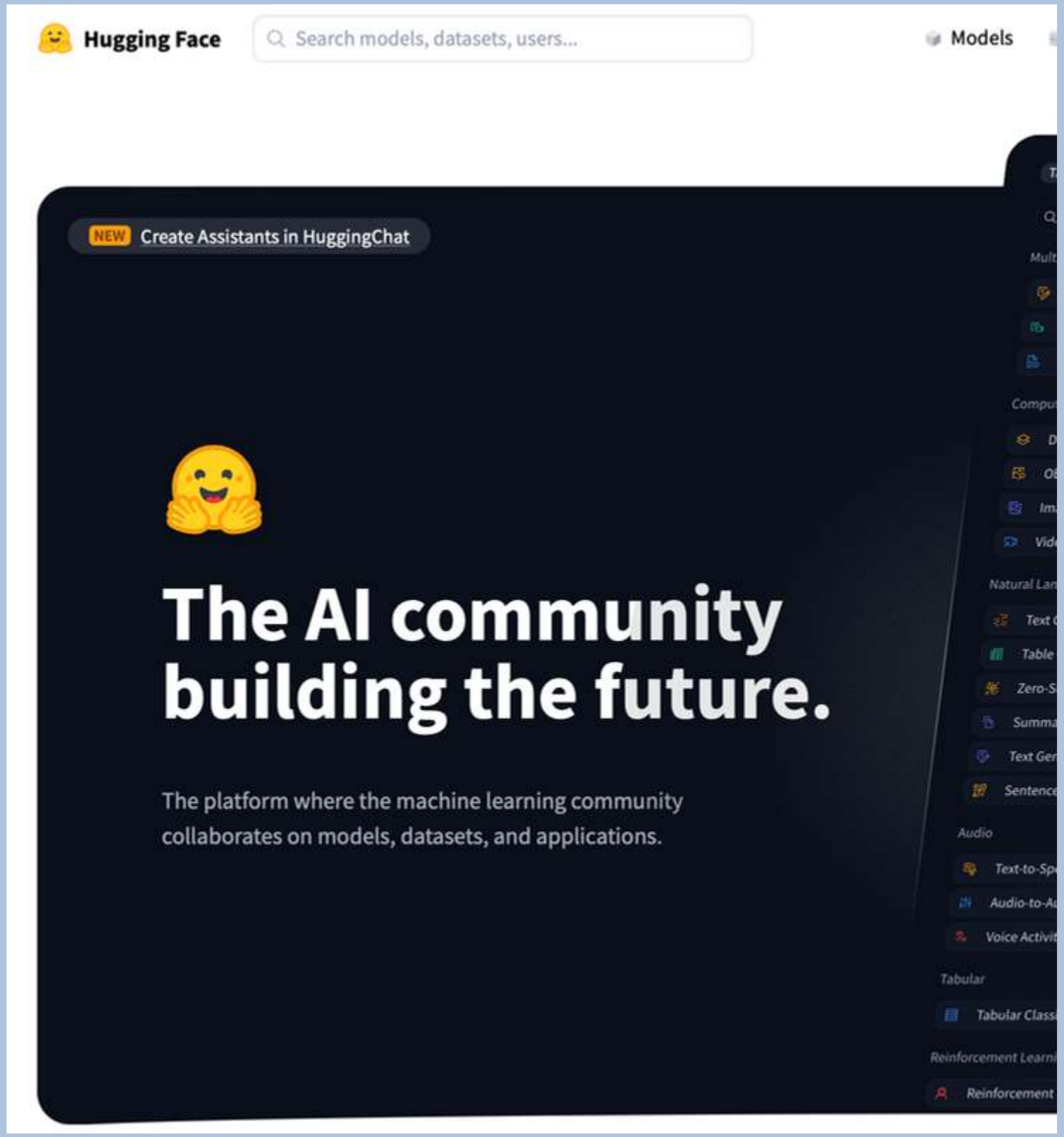
# Community data and models

**Les Houches guide to reusable ML models in LHC analyses**

*Jack Y. Araz[1], Andy Buckley[2], Gregor Kasieczka[3], Jan Kieseler[4], Sabine Kraml[5], Anders Kvellestad[6], Andre Lessa[7], Tomasz Procter[2], Are Raklev[6], Humberto Reyes-Gonzalez[8,9,10], Krzysztof Rolbiecki[11], Sezen Sekmen[12], Gokhan Unel[13]*



## Model Card

- **Model Details**. Basic information about the model.
  - Person or organization developing model
  - Model date
  - Model version
  - Model type
  - Information about training algorithms, parameters, fairness constraints or other applied approaches, and features
  - Paper or other resource for more information
  - Citation details
  - License
  - Where to send questions or comments about the model
- **Intended Use**. Use cases that were envisioned during development.
  - Primary intended uses
  - Primary intended users
  - Out-of-scope use cases
- **Factors**. Factors could include demographic or phenotypic groups, environmental conditions, technical attributes, or others listed in Section 4.3.
  - Relevant factors
  - Evaluation factors
- **Metrics**. Metrics should be chosen to reflect potential real-world impacts of the model.
  - Model performance measures
  - Decision thresholds
  - Variation approaches
- **Evaluation Data**. Details on the dataset(s) used for the quantitative analyses in the card.
  - Datasets
  - Motivation
  - Preprocessing
- **Training Data**. May not be possible to provide in practice. When possible, this section should mirror Evaluation Data. If such detail is not possible, minimal allowable information should be provided here, such as details of the distribution over various factors in the training datasets.
- **Quantitative Analyses**
  - Unitary results
  - Intersectional results
- **Ethical Considerations**
- **Caveats and Recommendations**

# Model Cards for Model Reporting

Margaret Mitchell, Simone Wu, Andrew Zaldivar, Parker Barnes, Lucy Vasserman, Ben Hutchinson, Elena Spitzer, Inioluwa Deborah Raji, Timnit Gebru
{mmitchellai,simonewu,andrewzaldivar,parkerbarnes,lucyvasserman,benhutch,espitzer,tgebru}@google.com
deborah.raji@mail.utoronto.ca

openai/**gpt-3**

GPT-3: Language Models are Few-Shot Learners

| 4 | 21 | 16k | 2k |
|---|---|---|---|
| Contributors | Used by | Stars | Forks |

**gpt-3/model-card.md at master · openai/gpt-3**

GPT-3: Language Models are Few-Shot Learners. Contribute to openai/gpt-3 development by creating an account on GitHub.

GitHub

# Roadmap for ML in Nuclear Science

## 2020 AI for Nuclear Physics workshop Community Identified Needs and Commonalities:

- Workforce development
  - educational activities
  - community: centralized, value interdisciplinary work
  - collaboration with ML community
- Uncertainty quantification
- appropriate use of industry-standard tools
- problem-specific tools
- comprehensive data management
- adequate computational resources

Jefferson Lab

Group photo from the workshop AI for Nuclear Physics held at Thomas Jefferson National Accelerator Facility on March 4-6, 2020.

# THANK YOU!

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