The NSF AI Institute for Artificial Intelligence and Fundamental Interactions

Jesse Thaler

IAIFI Director



High Energy Physics Advisory Panel — December 4, 2020

NSF: National AI Research Institutes

5 Inaugural Institutes:

+2 USDA-NIFA Institutes

NSF AI Institute for Research on Trustworthy AI in Weather, Climate, and Coastal Oceanography

NSF AI Institute for Foundations of Machine Learning

NSF AI Institute for Student-AI Teaming

NSF AI Institute for Molecular Discovery, Synthetic Strategy, and Manufacturing

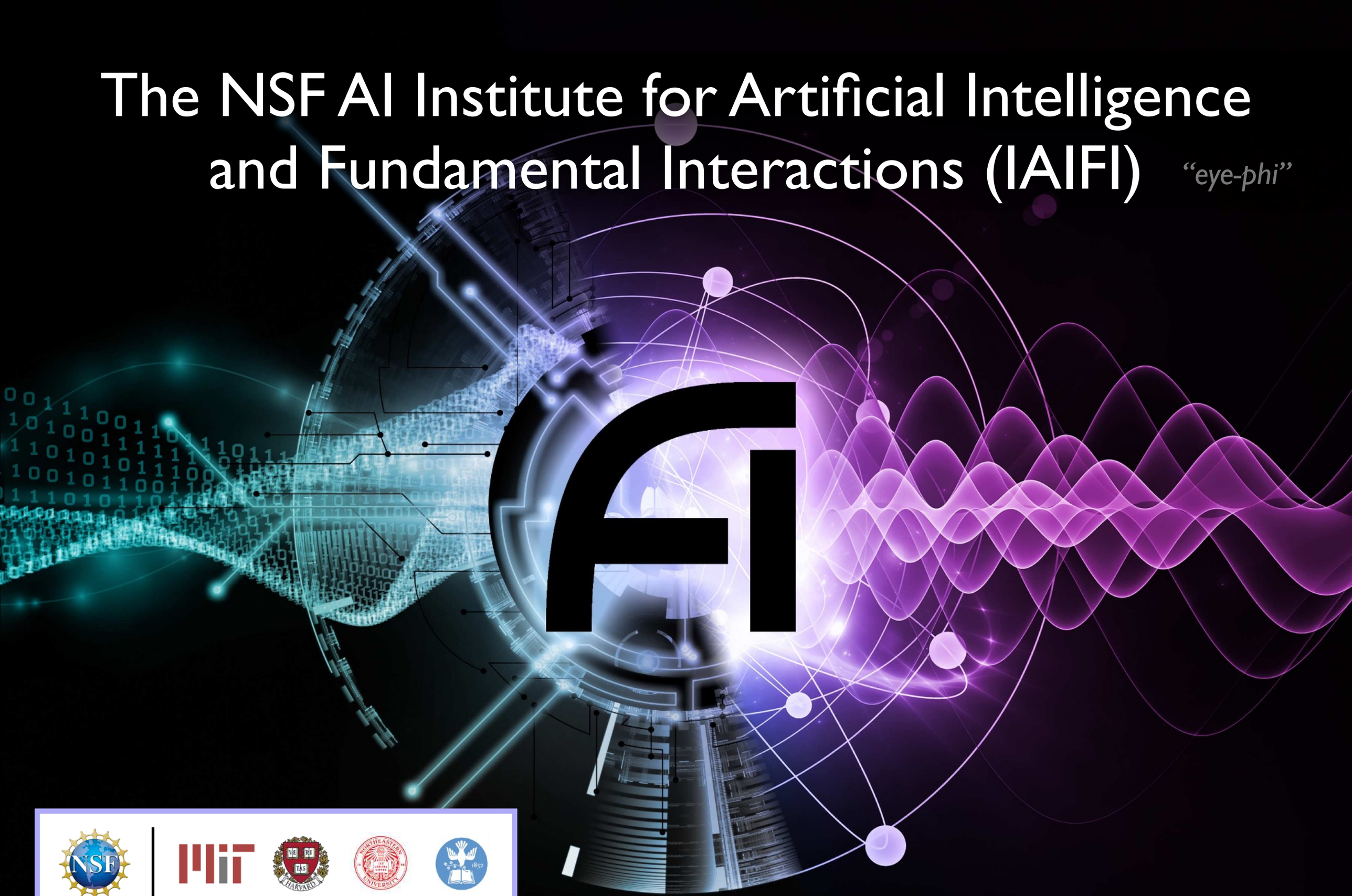
NSF AI Institute for Artificial Intelligence and Fundamental Interactions

8 Themes for Next Round:

Human-AI Interaction and Collaboration
AI Institute for Advances in Optimization
AI and Advanced Cyberinfrastructure
Advances in AI and Computer and Network Systems
AI Institute in Dynamic Systems
AI-Augmented Learning
AI to Advance Biology
AI-Driven Innovation in Agriculture and the Food System

[NSF Announcement, August 26, 2020; Call for New Proposals]

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI) *"eye-phi"*



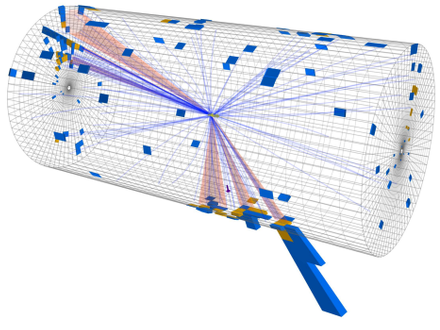
[http://iaifi.org/, MIT News Announcement]

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI) *"eye-phi"*

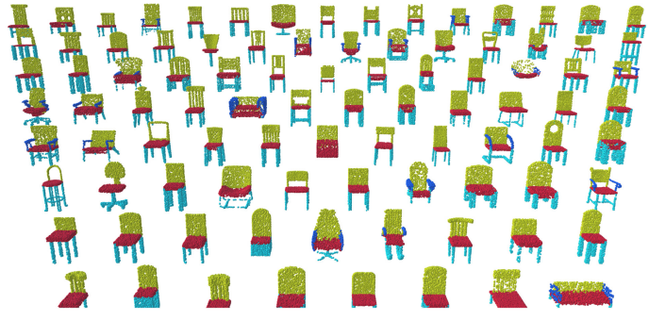
Advance physics knowledge — from the smallest building blocks of nature to the largest structures in the universe — and galvanize AI research innovation

Training, education & outreach at Physics/AI intersection
Cultivate early-career talent (e.g. IAIFI Fellows)
Foster connections to physics facilities and industry
Build strong multidisciplinary collaborations
Advocacy for shared solutions across subfields

E.g. Analyzing Collision Debris ⇔ Geometric Data Processing



[Harris, Schwartz, JDT, Williams]



[Wang, Sun, Liu, Sarma, Bronstein, Solomon, TOG 2019]

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI) *"eye-phi"*

Senior Investigators: 20 Physicists + 7 AI Experts + IAIFI Affiliates

Junior Investigators: ≈20 PhD Students, ≈7 IAIFI Fellows in steady state

MIT

Pulkit Agrawal
Lisa Barsotti
Isaac Chuang
William Detmold
Bill Freeman
Philip Harris
Kerstin Perez
Alexander Rakhlin
Phiala Shanahan
Tracy Slatyer
Marin Soljacic
Justin Solomon
Washington Taylor
Max Tegmark
Jesse Thaler
Mike Williams

Harvard

Demba Ba
Edo Berger
Cora Dvorkin
Daniel Eisenstein
Doug Finkbeiner
Matthew Schwartz
Yaron Singer
Todd Zickler

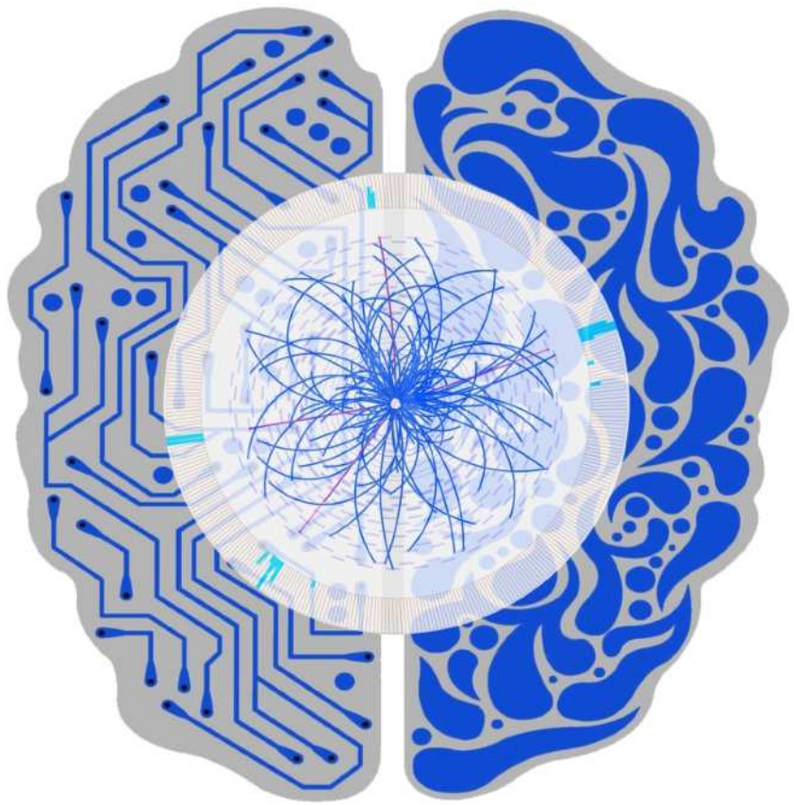
Northeastern University

James Halverson
Brent Nelson

Taritree Wongjirad

Boston Area: Critical Mass for Transformative Research in "Ab Initio AI"

Heavy HEP involvement across experiment, phenomenology & theory



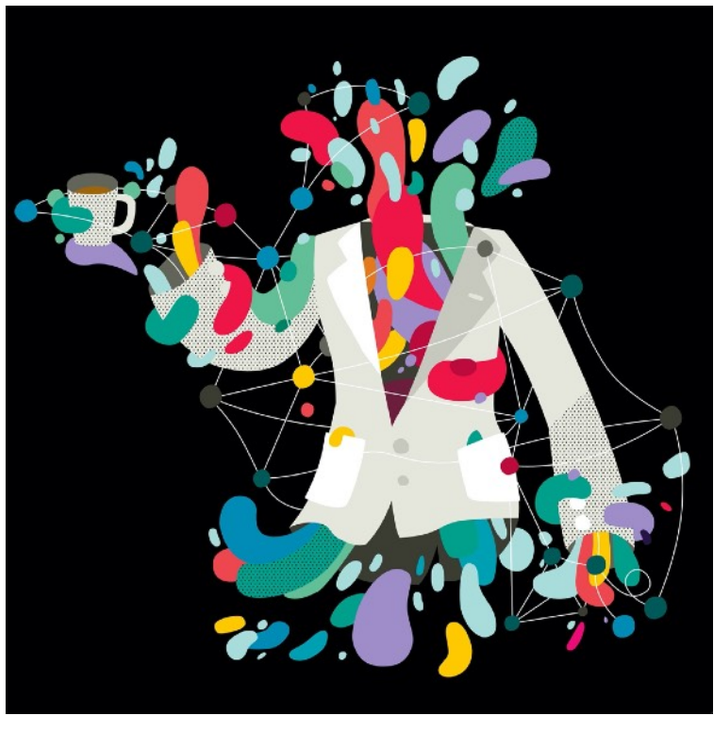
Can we teach a machine to "think" like a physicist?

(Have you ever tried to reason with a toddler?)

The New York Times

By Dennis Overbye Nov. 23, 2020

Can a Computer Devise a Theory of Everything?



The IAIFI Vision

Deep Learning meets Deep Thinking

Sophisticated networks, increased computational power & large data sets have led to extraordinary advances

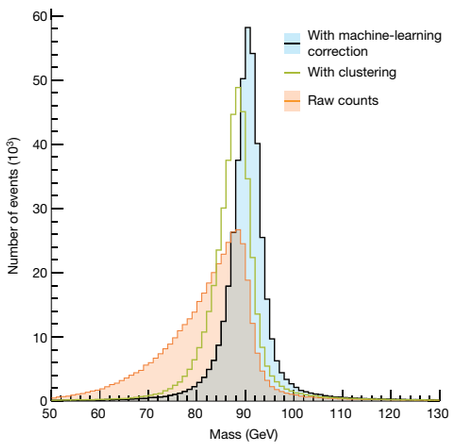
Continued progress requires exploiting the structure of physics problems & time-tested strategies of physical reasoning

"Deeper understanding, not just deeper networks"

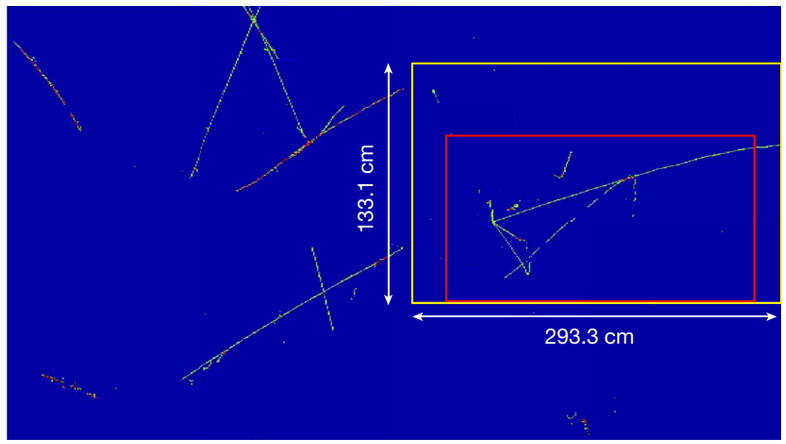
Extensive Use of ML in HEP

(backup slide from my May 2019 HEPAP talk)

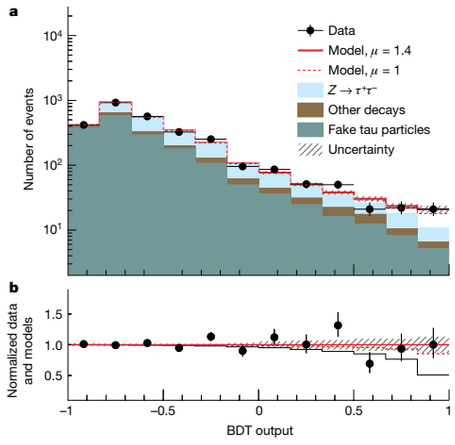
CMS: $Z \to e^+e^-$ calibration



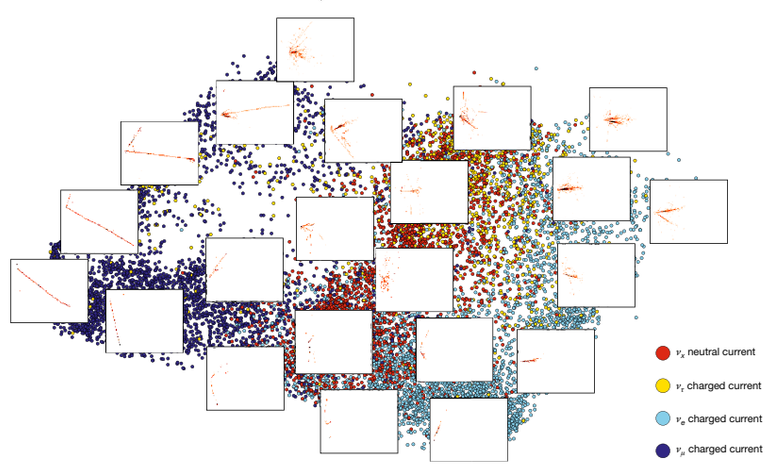
MicroBooNE: Object Identification



ATLAS: $H \to \mu^+\mu^-$ search



NOvA: Object Classification



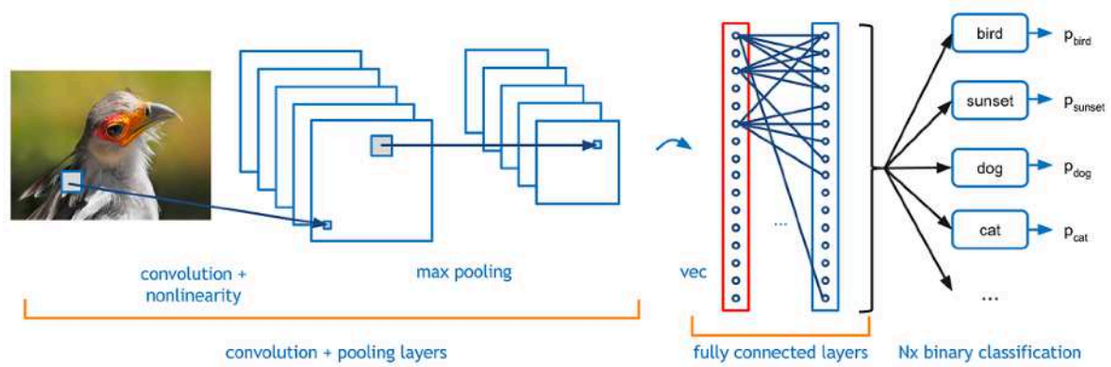
Machine learning is transforming many aspects of society, including fundamental physics research

[figures from Radovic, **Williams**, Rousseau, Kagan, Bonacorsi, Himmel, Aurisano, Terao, **Wongjirad**, Nature 2018]

Off-the-Shelf ML for HEP?

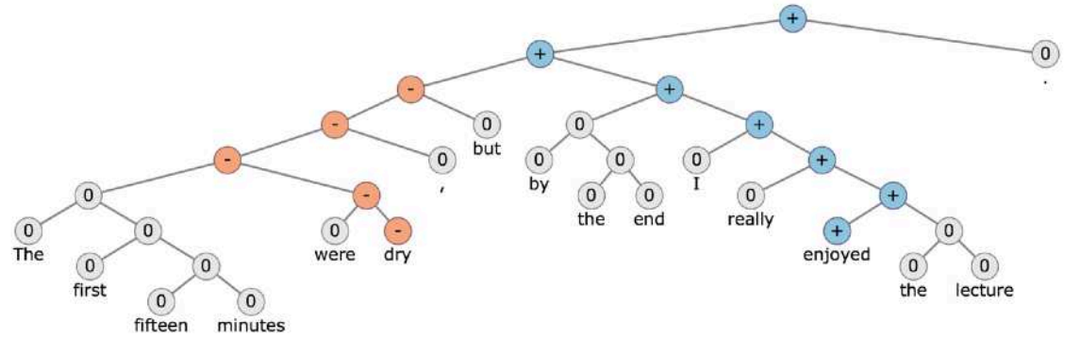
2D Images?

Appropriate for fixed-grid calorimeters,
but less ideal for tracking detectors



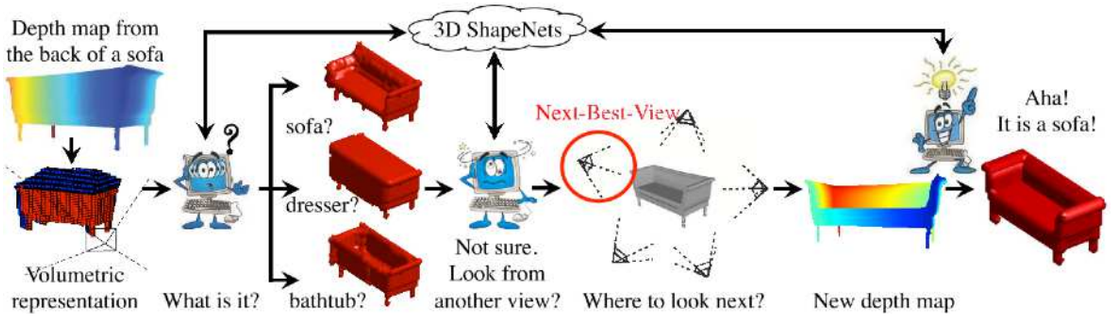
Natural Language?

Clustering can yield "semantic" structure, but
identical particles have no intrinsic ordering



3D Objects?

Much closer to particle physics,
though doesn't capture all symmetries



AI²: Ab Initio Artificial Intelligence

Machine learning that incorporates
first principles, best practices, and domain knowledge
from fundamental physics

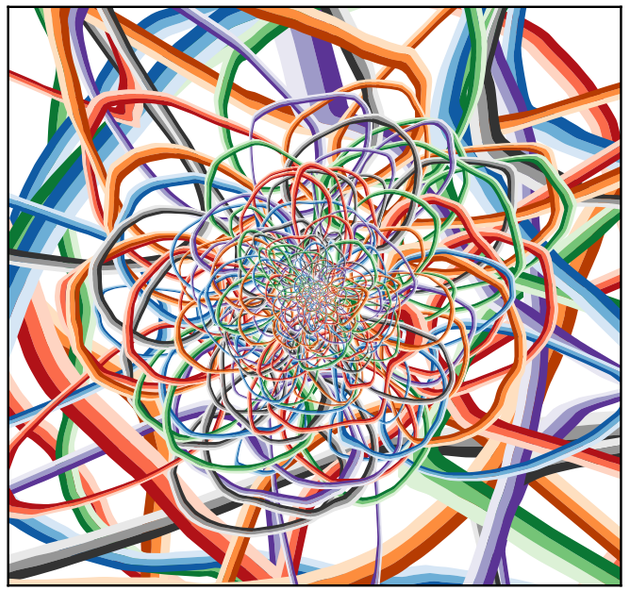
Symmetries, conservation laws, scaling relations, limiting behaviors, locality, causality, unitarity, gauge invariance, entropy, least action, factorization, unit tests, exactness, systematic uncertainties, reproducibility, verifiability, …

AI²: Ab Initio Artificial Intelligence

Convolutional Neural Networks ⇔ Translational Equivariance

⇒ Momentum Conservation

Energy Flow Networks ⇔ Identical Particles (QM)
Infrared/Collinear Safety (QFT)



[Komiske, Metodiev, JDT, JHEP 2019]

AI Powerful strategy to analyze LHC collisions

× **AI** Efficient neural network for point clouds

= **AI²** Shared solution across disciplines

Progress driven by early-career talent with cross-disciplinary expertise:

IAIFI Postdoctoral Fellowships

Recruit and train a talented and diverse group of early-career researchers
Spark interdisciplinary, multi-investigator, multi-subfield collaborations

Physics Theory

Physics Experiment

AI Foundations

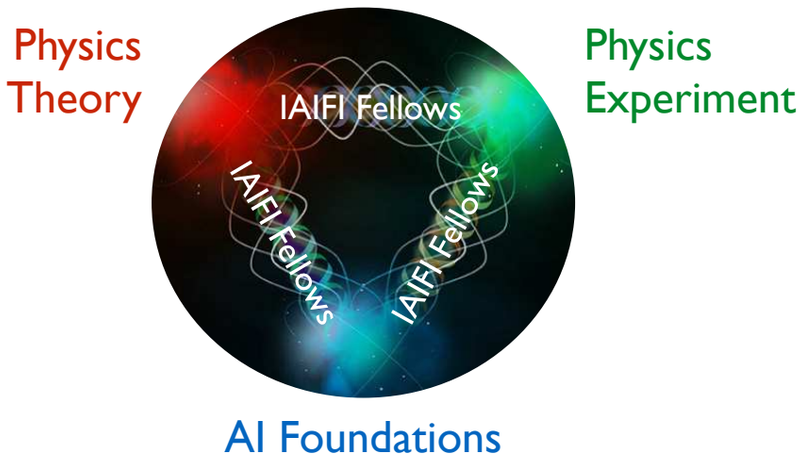
133 applicants for 2021–2024 IAIFI Fellows

[https://iaifi.org/fellows.html; https://academicjobsonline.org/ajo/jobs/16695]

IAIFI Research Plan

AI² for Theoretical Physics

Standard Model of Nuclear & Particle Physics
String Theory & Physical Mathematics
Astroparticle Physics
Automated Discovery of Physics Models



AI² for Experimental Physics

Particle Physics Experiments
Gravitational Wave Interferometry
(Multi-Messenger) Astrophysics

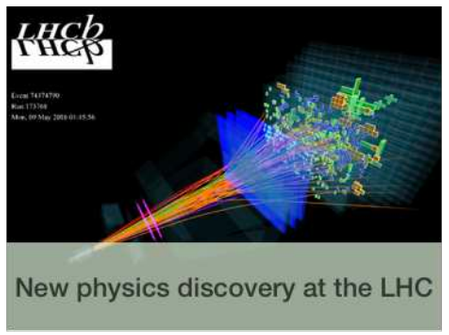
AI² for Foundational AI

Symmetries & Invariance
Speeding up Control & Inference
Physics-Informed Architectures
Neural Networks Theory

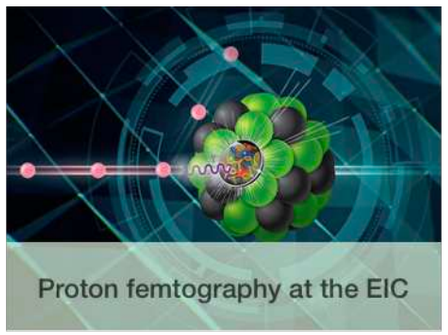
AI² for Theoretical Physics

E.g. Lattice Field Theory for Nuclear/Particle Physics

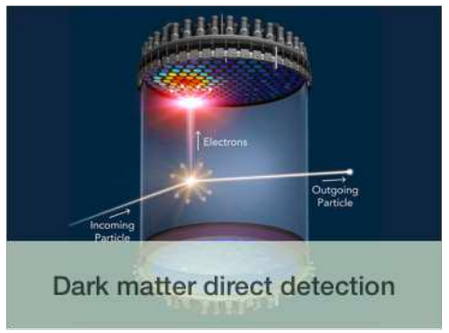
Equations governing the strong nuclear force are known, but precision computations are extremely demanding (>10% of open supercomputing in US)



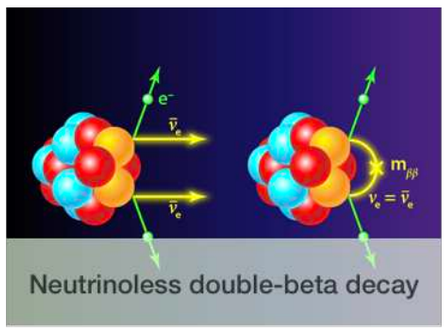
New physics discovery at the LHC



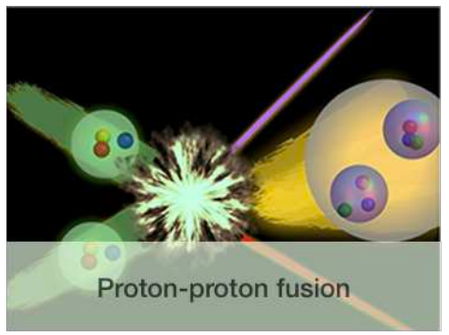
Proton femtography at the EIC



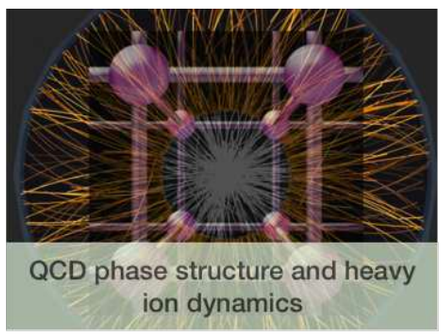
Dark matter direct detection



Neutrinoless double-beta decay



Proton-proton fusion



QCD phase structure and heavy ion dynamics

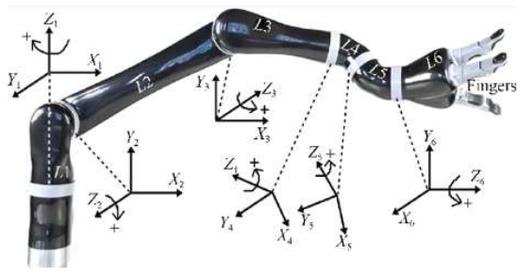
Industry collaboration to develop custom AI tools

Google DeepMind Massachusetts Institute of Technology

Custom generative models based on normalizing flows achieve 1000-fold acceleration while preserving symmetries & guaranteeing exactness

Tools designed for physics find interdisciplinary applications

Robotics



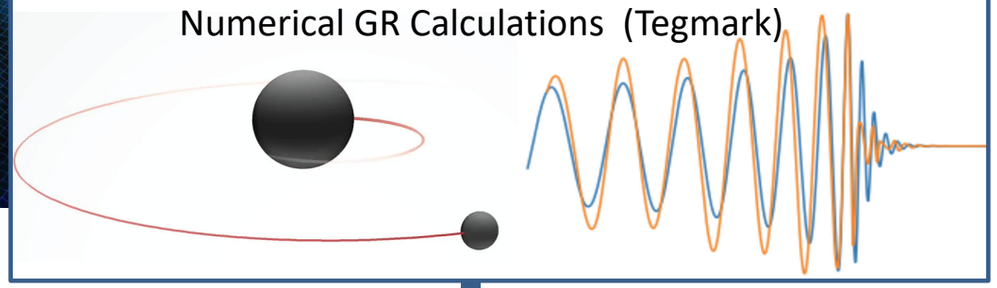
[Kanwar, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, **Shanahan**, PRL 2020]

AI² for Experimental Physics

E.g. Gravitational Wave Interferometry at LIGO

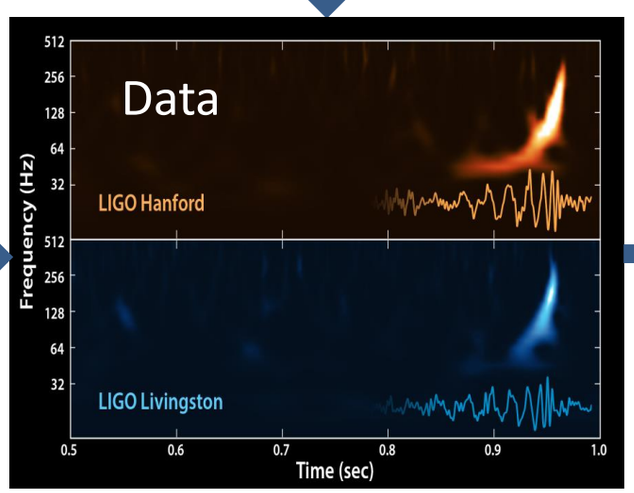
Potential to enhance the physics potential of flagship experiments via improved calibrations, better quantification of uncertainties, enhanced interpretability, and sub-microsecond inference

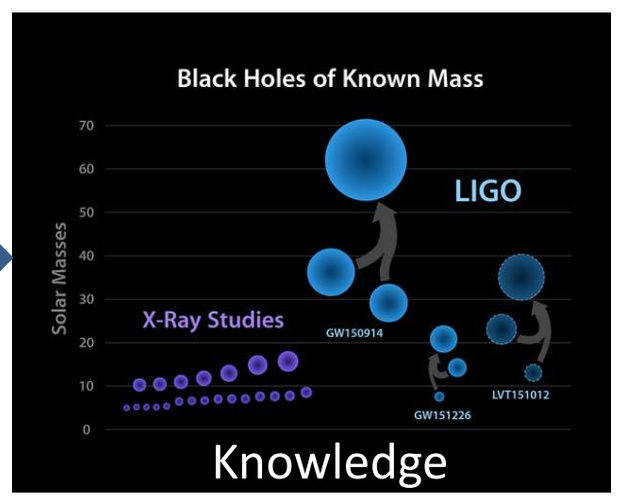
Theory Inputs: AI² to Speed Up Numerical GR Calculations (Tegmark)



LHC Fast-ML to speed up multi-messenger astrophysics (Harris)

Autoencoders improve LIGO's sensitivity by 20% [2005.06534]





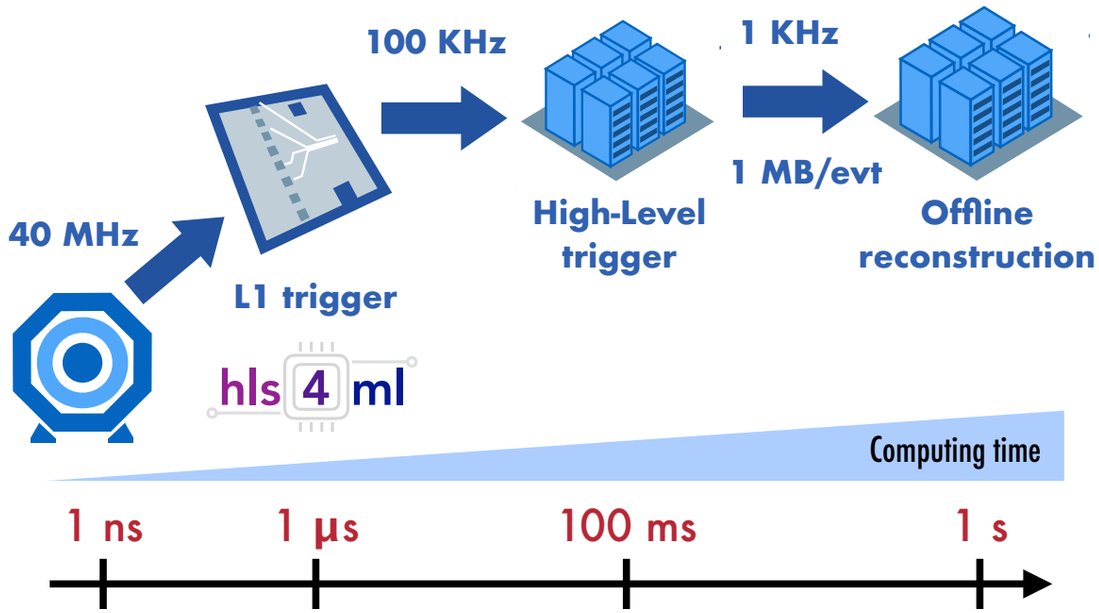
Propose using RL for Noise Reduction (Barsotti, Rakhlin)

AI² for Experimental Physics

E.g. Gravitational Wave Interferometry at LIGO

Potential to enhance the physics potential of flagship experiments via improved calibrations, better quantification of uncertainties, enhanced interpretability, and sub-microsecond inference

Outgrowth of Sub-Microsecond Inference for LHC Triggering



[talk by Ngadiuba, Fast ML Workshop, Nov 30, 2020;
Duarte, Han, Harris, Jindariani, Kreinar, Kreis, Ngadiuba, Pierini, Rivera, Tran, Wu, JINST 2018]

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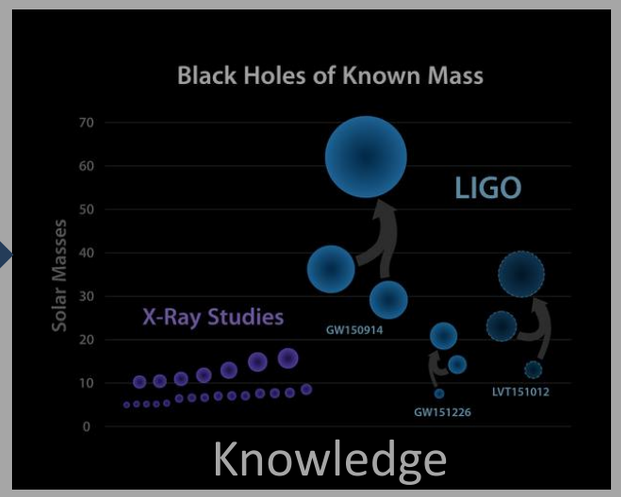


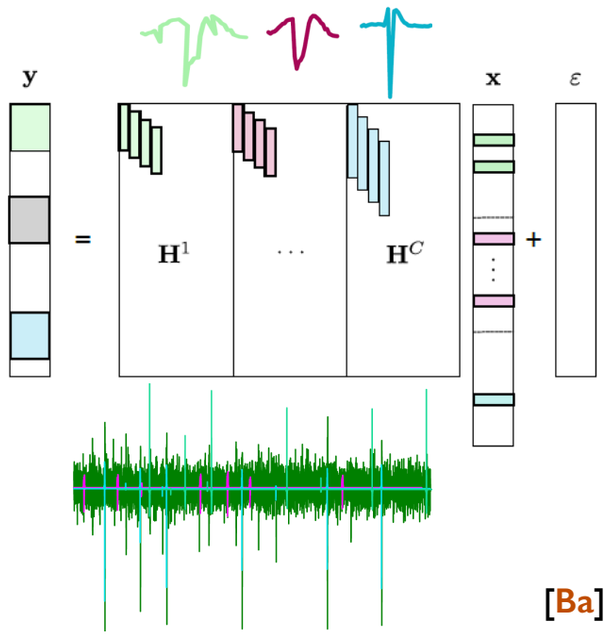
Rakhlin)

AI² for Foundational AI

E.g. Deconvolution Across Disciplines

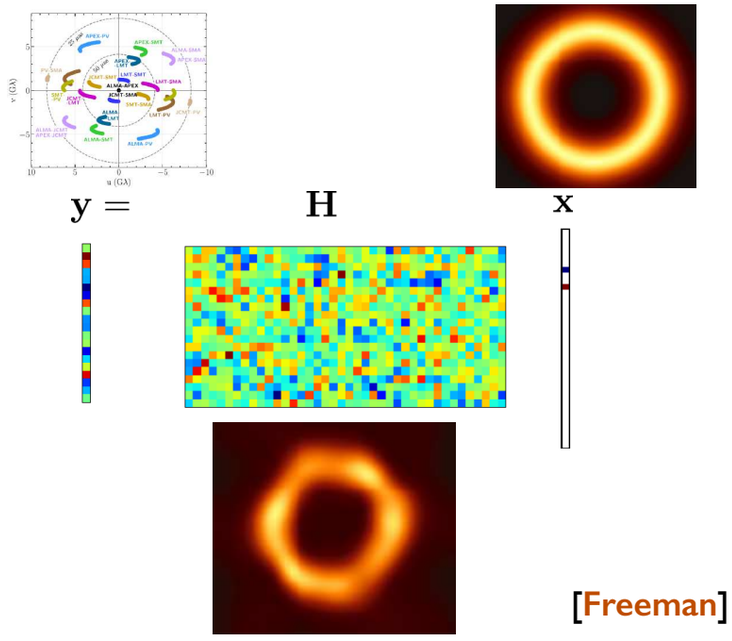
The unique features of physics applications and the power of physics principles offer compelling research opportunities to advance the field of AI research itself

Sparse Coding Networks and Neuronal Source Separation



[Ba]

Event Horizon Telescope and Black Hole Imaging

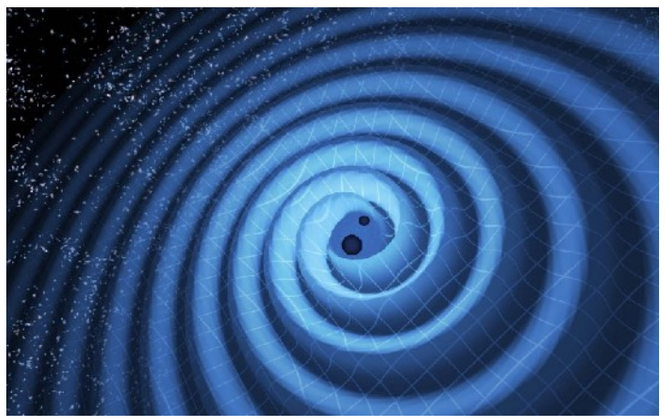


[Freeman]

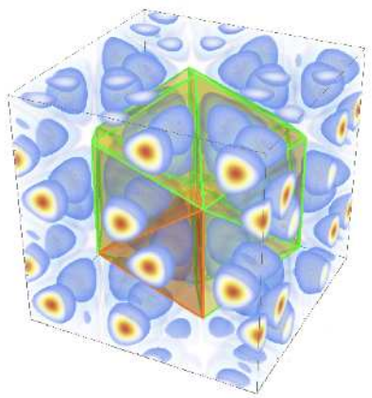
Highly relevant for HEP tasks ranging from detector unfolding to anomaly detection
Capitalize on physics priors and interpretability for improved robustness

Artificial Intelligence ⇔ *Fundamental Interactions*

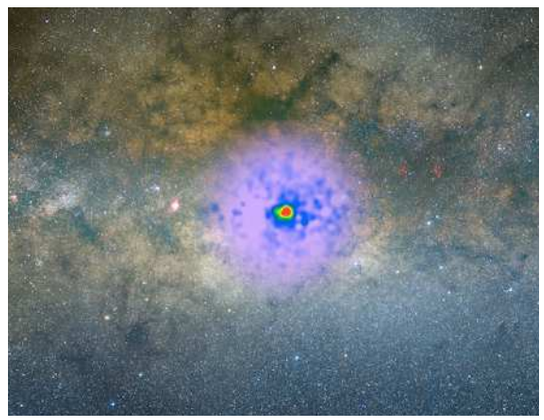
Gravitational Waves



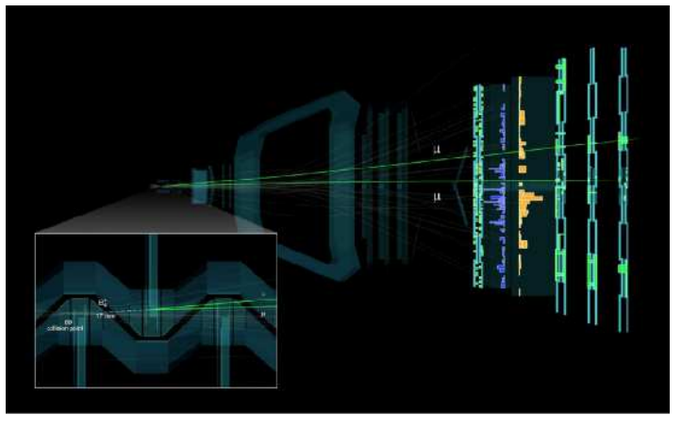
Nuclear Physics



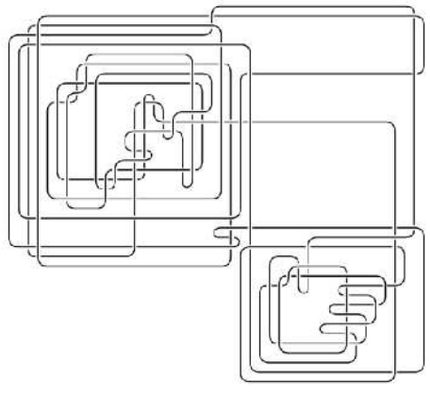
Astrophysics



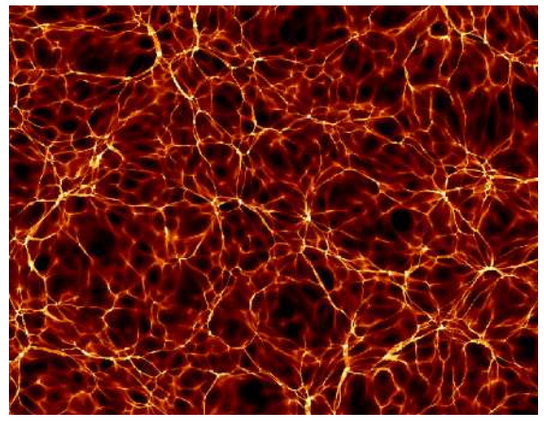
Particle Colliders



Mathematical Physics



Dark Matter



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IAIFI Activities & Synergies

Research Engagement

- Regular Internal Meetings
- External Seminar Speakers
- Long-term Visitor Program
- IAIFI Affiliates
- Annual IAIFI Workshop (Summer 2022)

Workforce Development

- IAIFI Postdoctoral Fellowship (Fall 2021)
- Cross-Disciplinary Mentoring
- Interdisciplinary PhD Program
- Annual PhD Summer School (Summer 2022)

Digital Learning

- Online Physics/AI Course Modules
- Expansion of MITx MicroMasters Program

Outreach

- IAIFI Podcasts
- K-12 Engagement
- Festivals & Museums

Broadening Participation

- Early Career & Equity Committee
- Summer Research Program
- MicroFellowship Program

Knowledge Transfer

- Summer Internship Placement
- CSAIL Alliances-like Program
- Joint Research Initiatives

Resources

- Shared Computing Resources
- Building 26 Penthouse Renovations

IAIFI Talking Points

IAIFI has a compelling vision for the future of Physics and AI research

Fuse "deep learning" revolution with time-tested strategies of "deep thinking" in physics
Gain deeper understanding of our universe and of principles underlying (machine) intelligence

IAIFI will train the next generation of researchers working at the intersection of Physics and AI

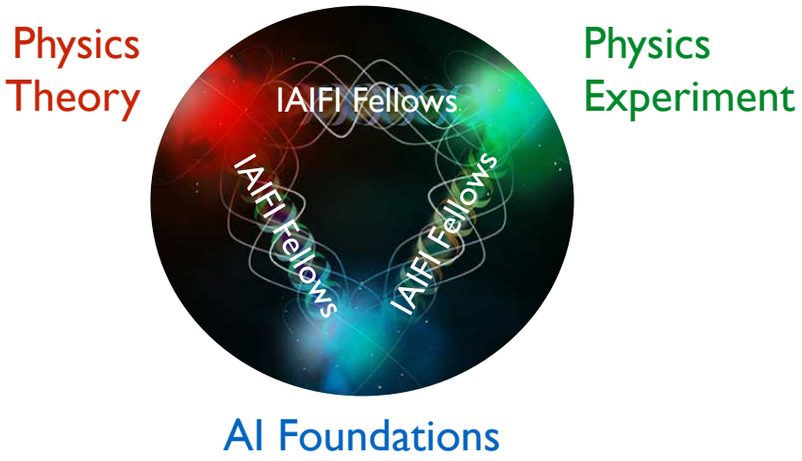
Programs like IAIFI Fellowships and Interdisciplinary PhD in Physics, Statistics & Data Science offer unique opportunities for early-career researchers to pursue their interests

IAIFI is part of a growing network of NSF AI Institutes, creating new opportunities for Physics-inspired research

HEP is a unique testbed for AI platforms, given the stringent requirements for verification, calibration, uncertainty handling, reproducibility, and speed

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI) *"eye-phi"*

Advance physics knowledge — from the smallest building blocks of nature to the largest structures in the universe — and galvanize AI research innovation



Training, education & outreach at Physics/AI intersection
Cultivate early-career talent (e.g. IAIFI Fellows)
Foster connections to physics facilities and industry
Build strong multidisciplinary collaborations
Advocacy for shared solutions across subfields

http://iaifi.org/

We look forward to collaborations and synergies with broader Physics + AI community