

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions

Jesse Thaler

IAIFI Director



AI+D Lunch Talk — September 11, 2020

NSF: National AI Research Institutes

*5 Inaugural
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]

Artificial Intelligence \leftrightarrow Fundamental Interactions



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

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI)

“eye-phi”



Senior Investigators: 20 Physicists + 7 AI Experts

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



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

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

James Halverson
Brent Nelson

The Northeastern University logo, featuring a red circular seal with the text "NORTHEASTERN UNIVERSITY" and "1898" around the perimeter, and "VERITAS VIRTUS" in the center.



Taritree Wongjirad

MIT c Boston Area: Critical Mass for Transformative Ab Initio AI Research

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI)

“eye-phi”

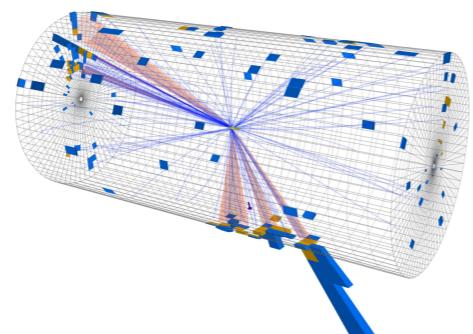


Advance physics knowledge — from the smallest building blocks of nature to the largest structures in the universe — and galvanize AI research innovation

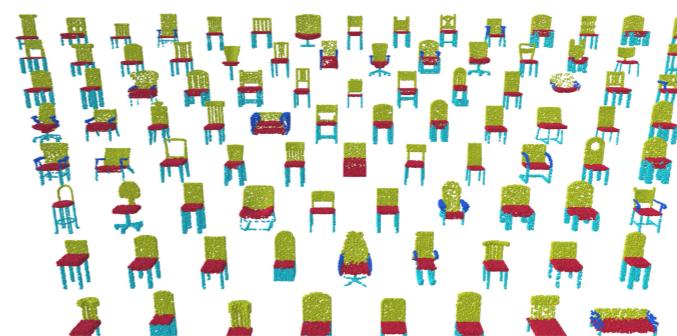


Training, education & outreach at Physics/AI intersection
Cultivate early-career talent (e.g. IAIFI Fellows)
Foster connections to physics facilities and industry
Build strong **multidisciplinary collaborations**
Advocacy for **shared solutions** across subfields

E.g. Analyzing Collision Debris \leftrightarrow Geometric Data Processing



[Harris, Schwartz, JDT, Williams]



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

“What is *Ab Initio Artificial Intelligence?*”

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

Deep Learning

Inpainting



Corrupted



Deep image prior

increased computational power and large data sets

[Ulyanov, Vedaldi, Lempitsky, CVPR 2018]

Deep Learning meets Deep Thinking

Inpainting



Corrupted



Deep image prior

Using randomly initialized neural network (!)

Progress made by understanding the structure of problems
(not just increased computational power and large data sets)

[Ulyanov, Vedaldi, Lempitsky, CVPR 2018]

The Rise of AI²: Ab Initio Artificial Intelligence

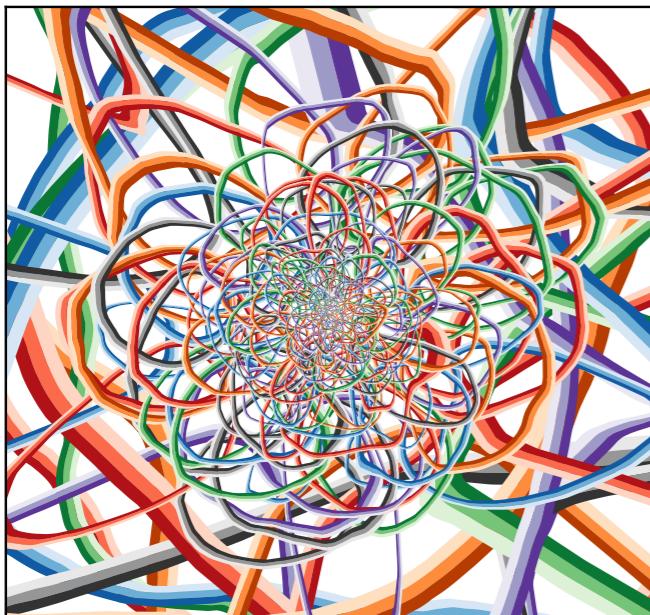
Machine learning that incorporates first principles, best practices, and domain knowledge from physics

Symmetries, conservation laws, scaling relations, limiting behaviors, locality, causality, unitarity, gauge invariance, factorization, unit tests, exactness, systematic uncertainties, ...

E.g.: Convolutional Neural Networks \Leftrightarrow Translational Equivariance

\Rightarrow Momentum Conservation

My research: Energy Flow Networks \Leftrightarrow Identical Particles (QM)
Infrared/Collinear Safety (QFT)



$$\begin{array}{c} \text{AI} \\ \times \text{AI} \\ = \text{AI}^2 \end{array}$$

Powerful and principled strategy to analyze collision debris at the Large Hadron Collider

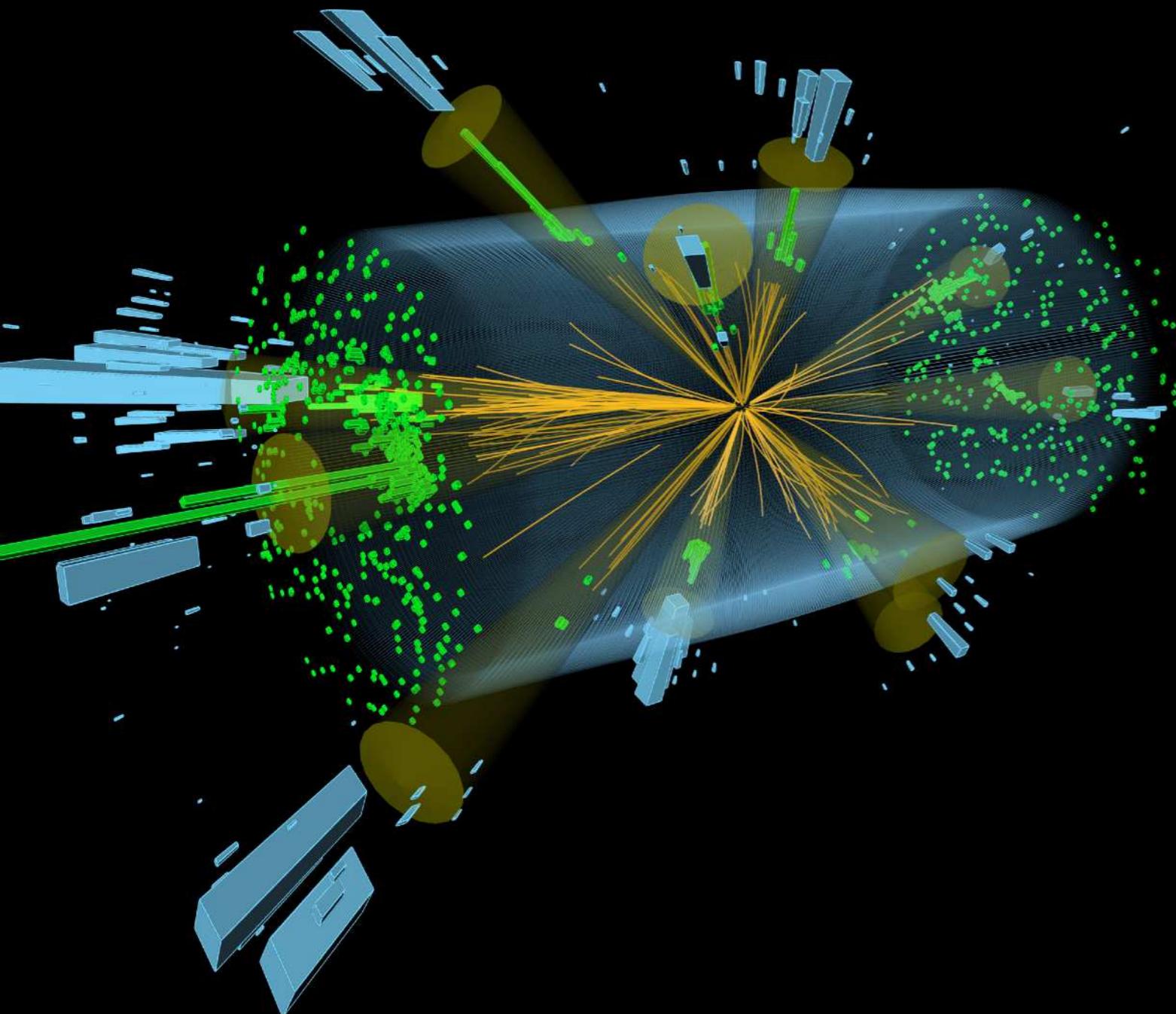
Efficient neural network for weighted point cloud classification, building off “deep sets”

Research that cuts across traditional disciplinary boundaries and generates shared solutions

[Komiske, Metodiev, *JDT, JHEP 2019*]

Collider Event with “Jets”

Collection of points in (momentum) space



T E H M

●	γ	photon
● ●	e^+	electron
● ● ● ●	μ^+	muon
● ● ●	π^+	pion
● ● ●	K^+	kaon
● ●	K_L^0	K-long
● ●	p/\bar{p}	proton
● ●	n/\bar{n}	neutron

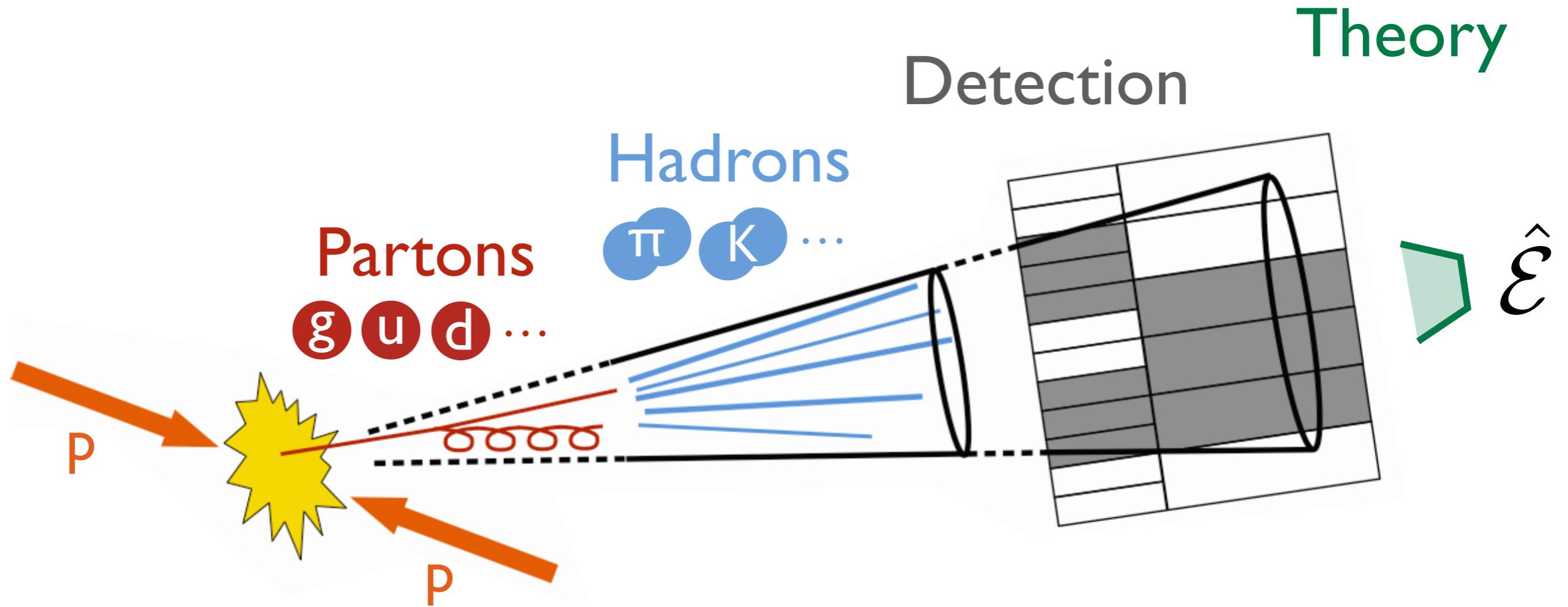
Point Cloud

Collection of points in (position) space



[Popular Science, 2013]

Dynamics of Jet Formation



Energy Flow:
Robust to hadronization and detector effects

$$\hat{\mathcal{E}} \simeq \lim_{t \rightarrow \infty} \hat{n}_i T^{0i}(t, vt\hat{n})$$

[see e.g. Sveshnikov, Tkachov, [PLB 1996](#); Hofman, Maldacena, [JHEP 2008](#); Mateu, Stewart, [JDT, PRD 2013](#); Belitsky, Hohenegger, Korchemsky, Sokatchev, Zhiboedov, [PRL 2014](#); Chen, Moult, Zhang, Zhu, [arXiv 2020](#)]

Introducing Energy Flow Networks



Symmetry:

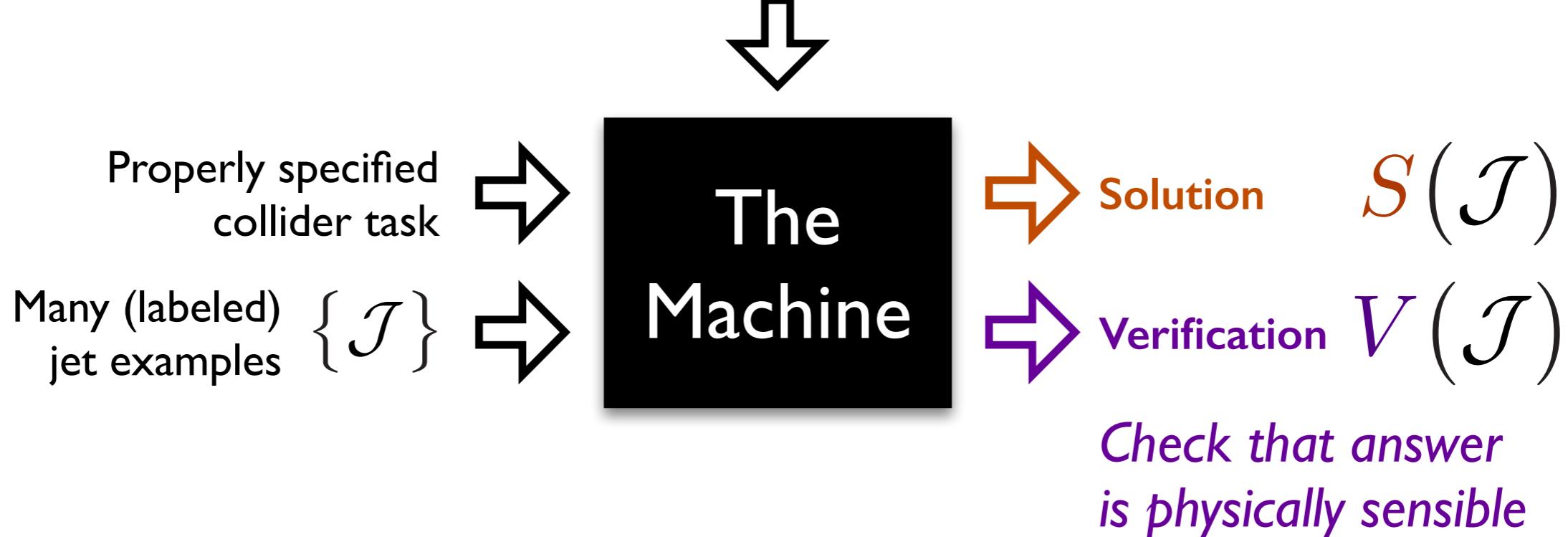
$$\mathcal{J} = \{ \vec{p}_1, \vec{p}_2, \vec{p}_3, \dots, \vec{p}_N \}$$

Unordered, Variable Length Set (QM!)

IRC Safety:

$$\vec{p} = \{ E, \hat{n}_x, \hat{n}_y, \hat{n}_z \}$$

Energy weighting (QFT!)

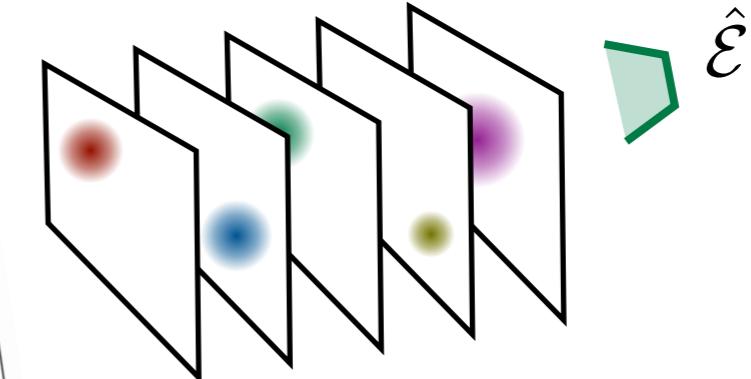
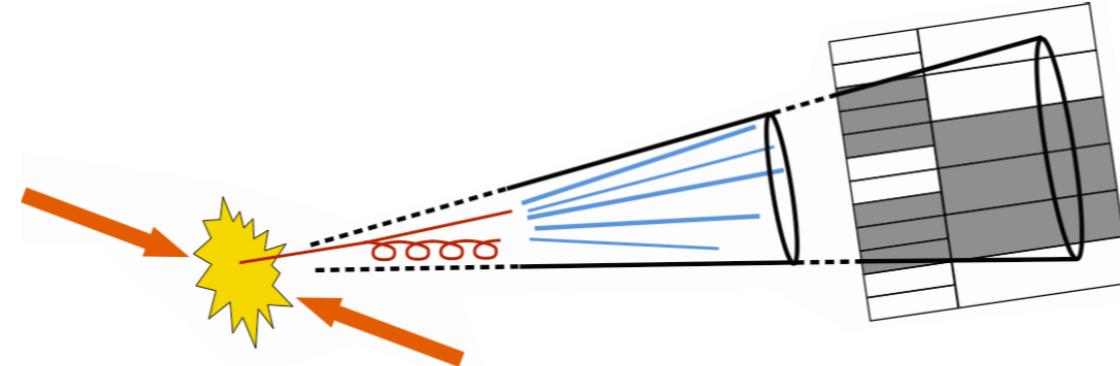


[<https://energyflow.network/>; Komiske, Metodiev, JDT, *JHEP* 2019; see also Komiske, Metodiev, JDT, *JHEP* 2018, *PRD* 2020; special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, *NIPS* 2017]

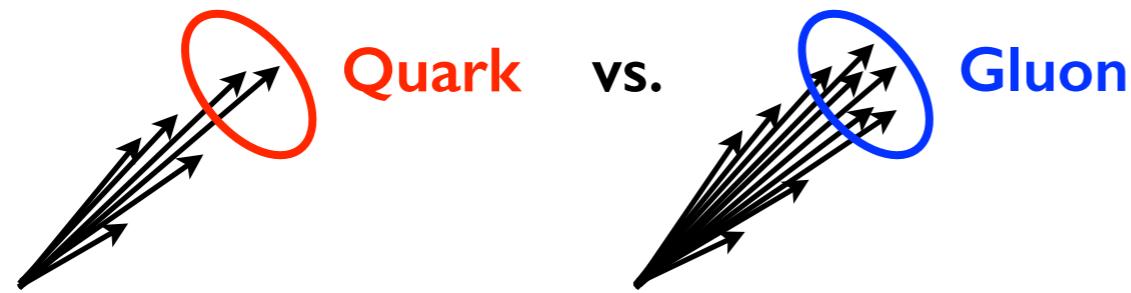
Introducing Energy Flow Networks



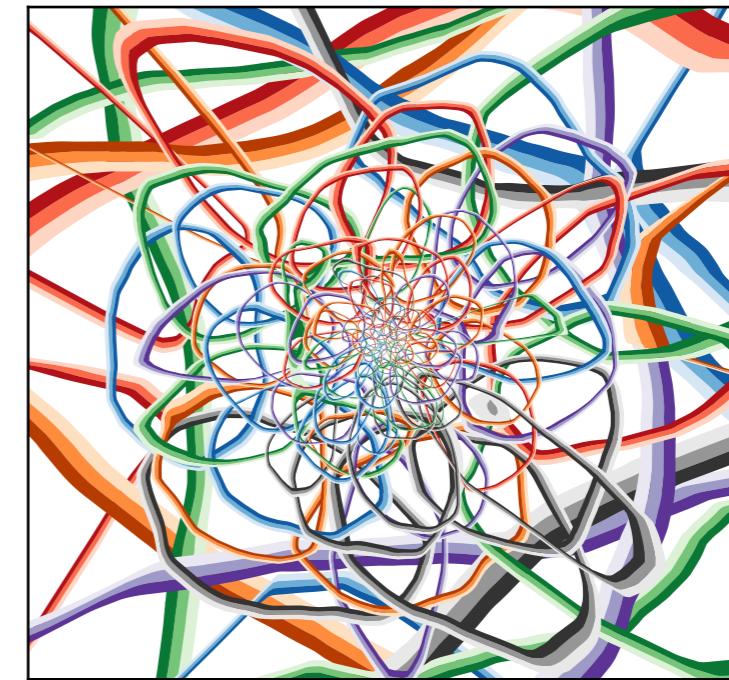
Visualization of EFN Latent Space:



“Hello, World!” of Jet Classification at LHC:

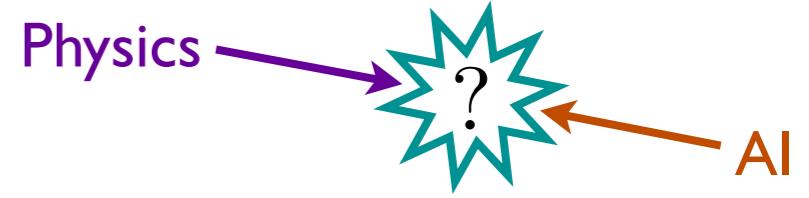


Learns the fractal structure of QCD!



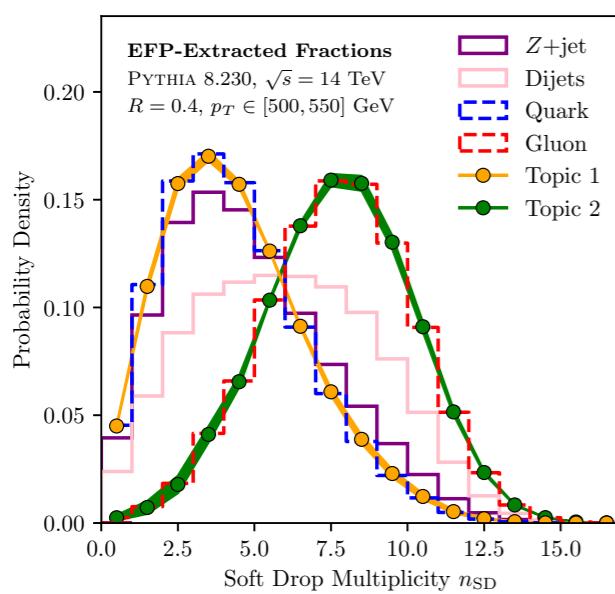
[<https://energyflow.network/>; Komiske, Metodiev, JDT, JHEP 2019; see also Komiske, Metodiev, JDT, JHEP 2018, PRD 2020; special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, NIPS 2017]

“Collision Course”



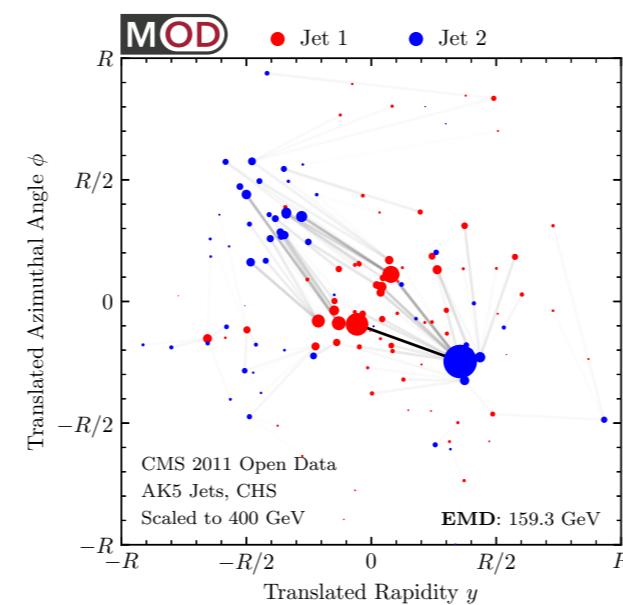
New insights into fundamental physics facilitated by advances in mathematics, statistics, and computer science (and vice versa!)

Quark/Gluon Definitions via Blind Source Separation



[Metodiev, JDT, [PRL 2018](#);
Komiske, Metodiev, JDT, [JHEP 2018](#)]

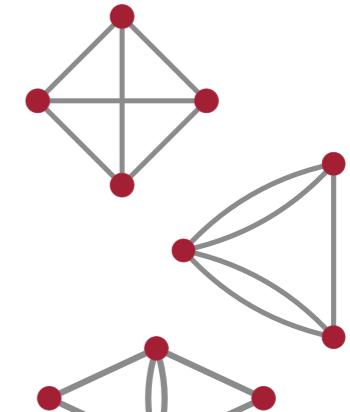
Half-Century of Collider Physics via Optimal Transport (!)



[Komiske, Metodiev, JDT, [PRL 2019](#), [JHEP 2020](#);
Komiske, Mastandrea, Metodiev, Naik, JDT, [PRD 2020](#)]

Kinematic Decomposition via Graph Theory

Edges d	Leafless Multigraphs	
	Connected A307317	All A307316
1	0	0
2	1	1
3	2	2
4	4	5
5	9	11
6	26	34
7	68	87
8	217	279
9	718	897
10	2 553	3 129
11	9 574	11 458
12	38 005	44 576
13	157 306	181 071
14	679 682	770 237
15	3 047 699	3 407 332
16	14 150 278	15 641 159



[Komiske, Metodiev, JDT,
[JHEP 2018](#), [PRD 2020](#)]

Driven by early-career talent with *cross-disciplinary expertise*:

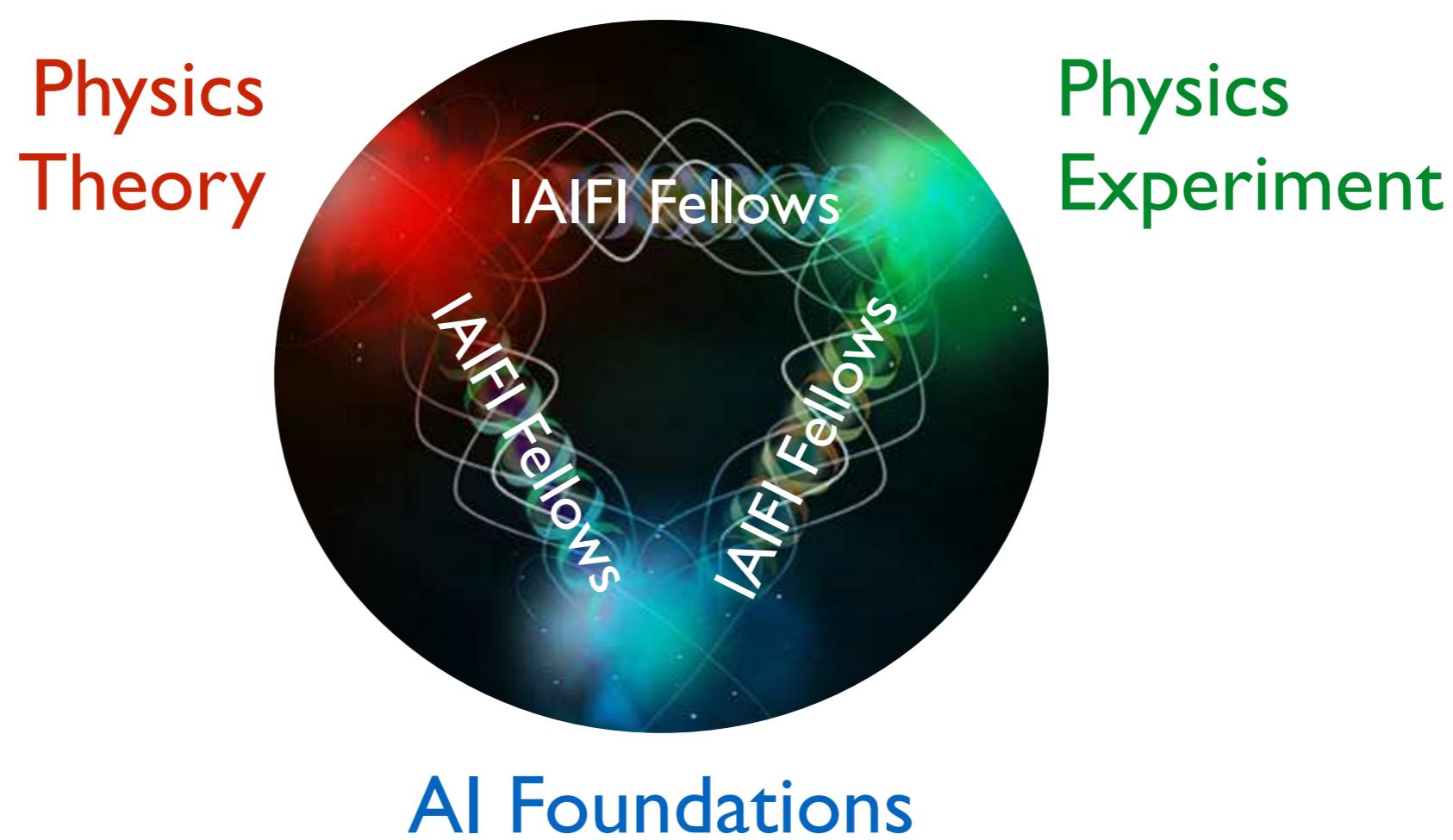


IAIFI Research Highlights, Proposed Activities & Synergies

IAIFI Postdoctoral Fellowships

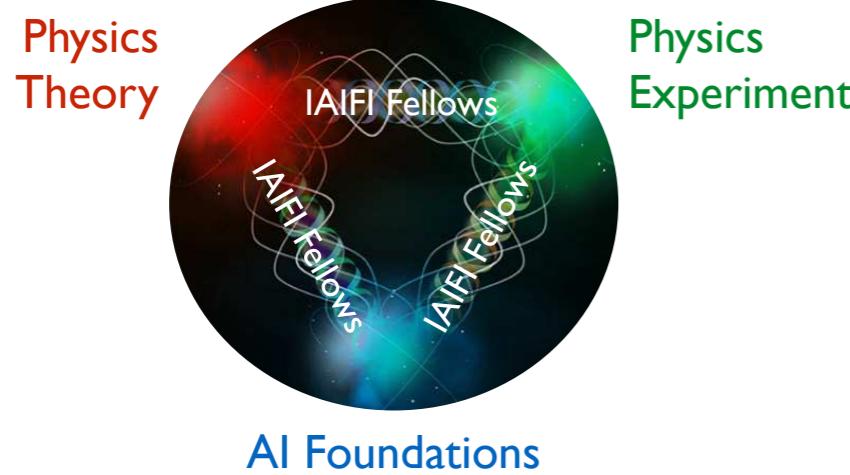


*Recruit and train a talented and diverse group of early-career researchers
Spark interdisciplinary, multi-investigator, multi-subfield collaborations*



2021–2024 application deadline: October 20, 2020

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



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

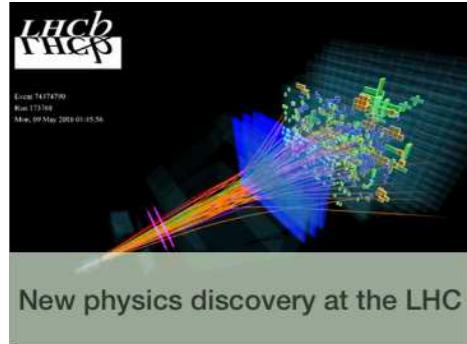
Symmetries & Invariance
Speeding up Control & Inference
Physics-Informed Architectures
Neural Networks Theory

AI² for Theoretical Physics

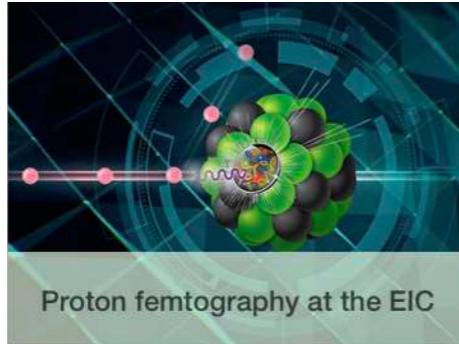


E.g. Lattice Field Theory for Nuclear/Particle Physics

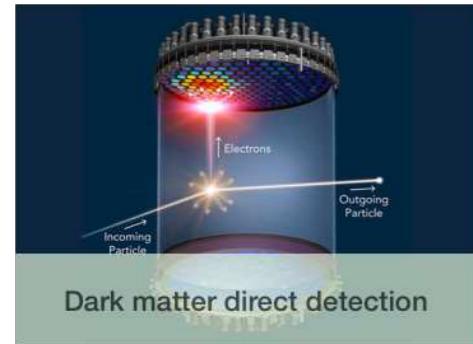
Equations governing the strong nuclear force are known, but precision computations are extremely demanding (>10% of open supercomputing in US)



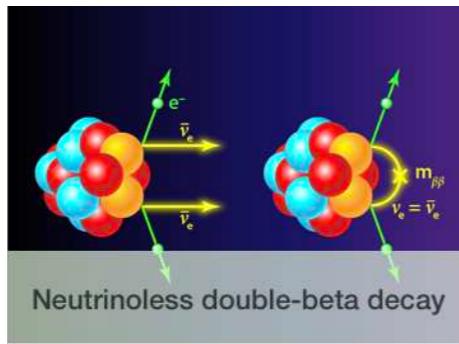
New physics discovery at the LHC



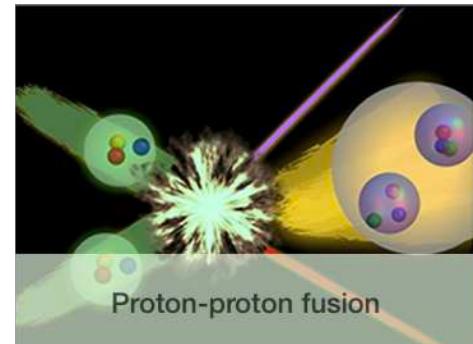
Proton femtography at the EIC



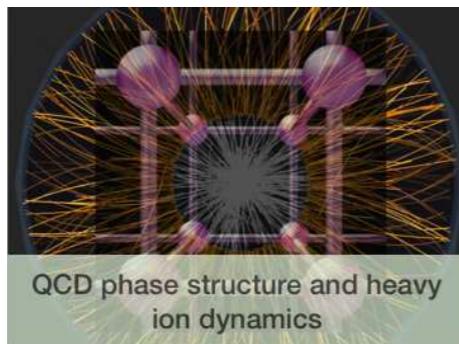
Dark matter direct detection



Neutrinoless double-beta decay



Proton-proton fusion



QCD phase structure and heavy ion dynamics

Industry collaboration to develop custom AI tools

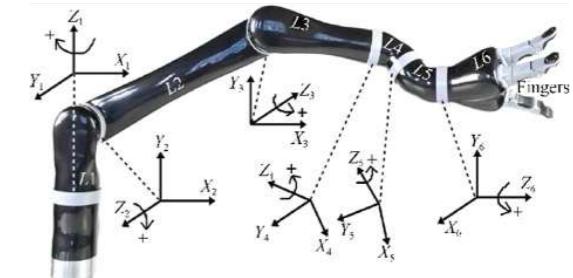


Massachusetts Institute of Technology

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

Tools designed for physics find **interdisciplinary applications**

Robotics



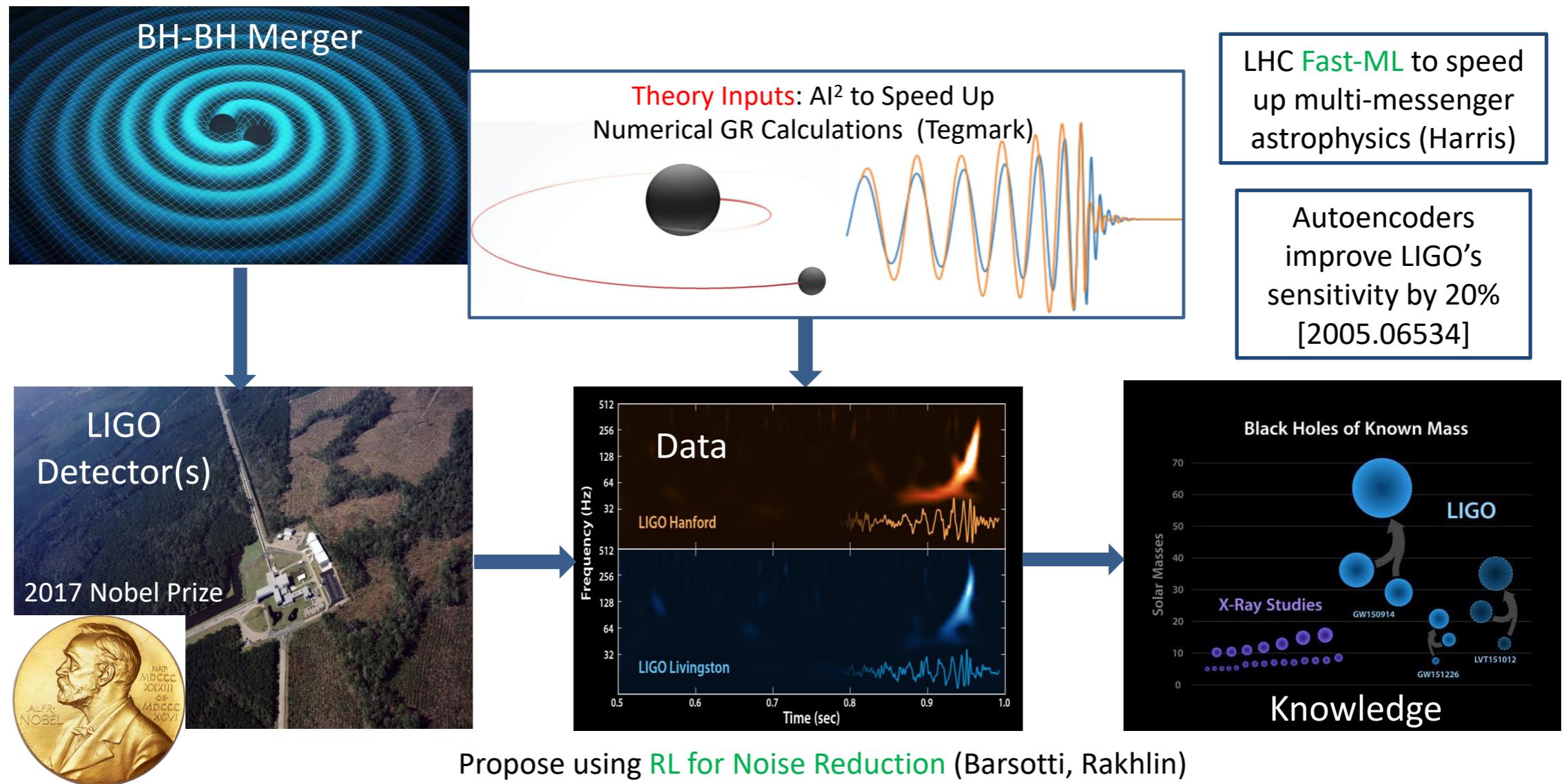
[Kanwar, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan, arXiv 2020]

AI² for Experimental Physics



E.g. Gravitational Wave Interferometry at LIGO

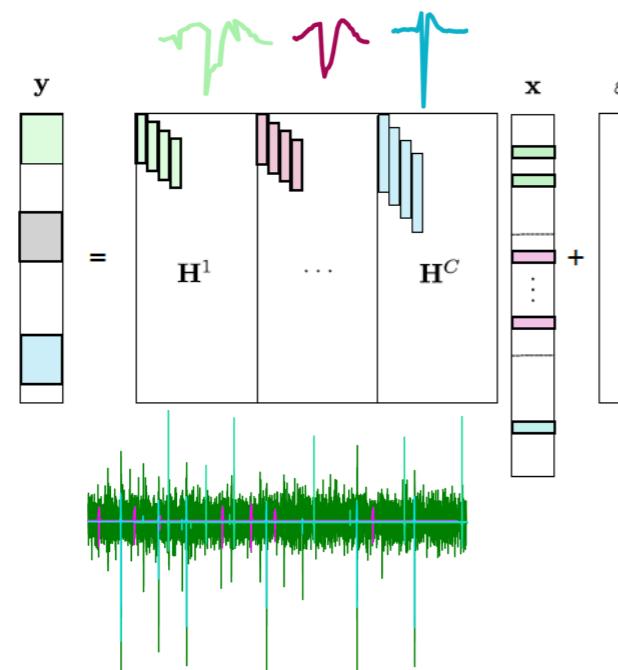
Potential to enhance the physics potential of flagship experiments via improved calibrations, better quantification of uncertainties, enhanced interpretability, and sub-microsecond inference



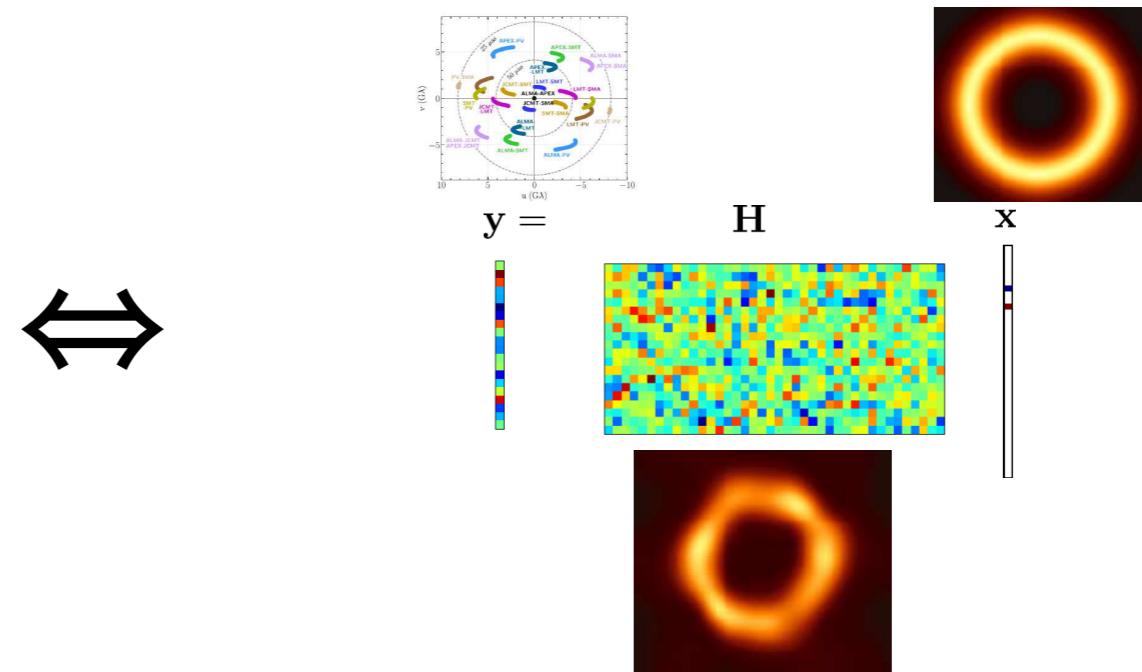
E.g. Deconvolution Across Disciplines

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)



*Capitalize on physics priors and interpretability for improved robustness
Leverage tools from physics to explain ability of networks to generalize*

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

*Places we can benefit
from AI+D experience*

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

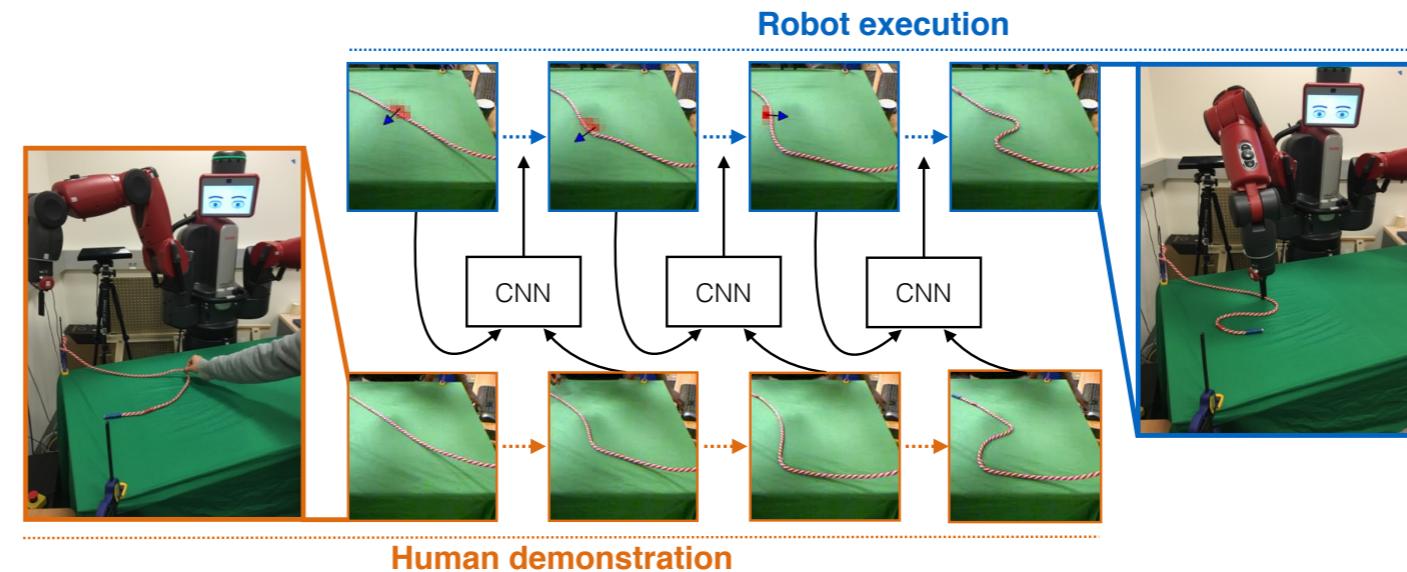
Resources

Shared Computing Resources

Building 26 Penthouse Renovations

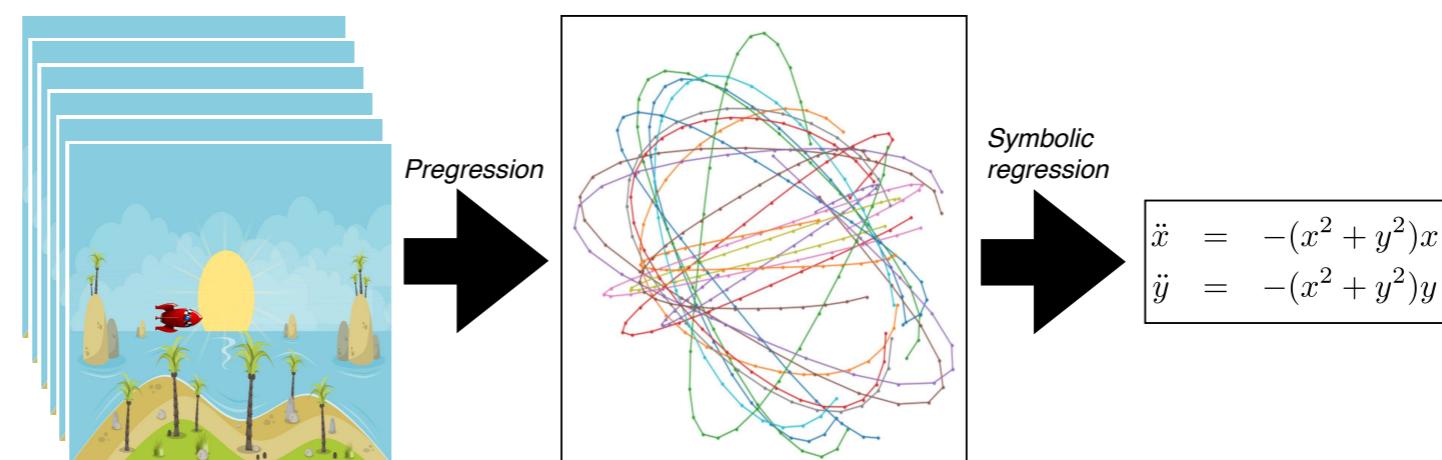
Learning Physical Laws from Spatiotemporal Data

*Course 6
Strategy:*



[Nair, Chen, **Agrawal**, Isola, Abbeel, Malik, Levine, ICRA 2017]

*Course 8
Strategy:*



[Udrescu, **Tegmark**, arXiv 2020]

IAIFI Activities & Synergies

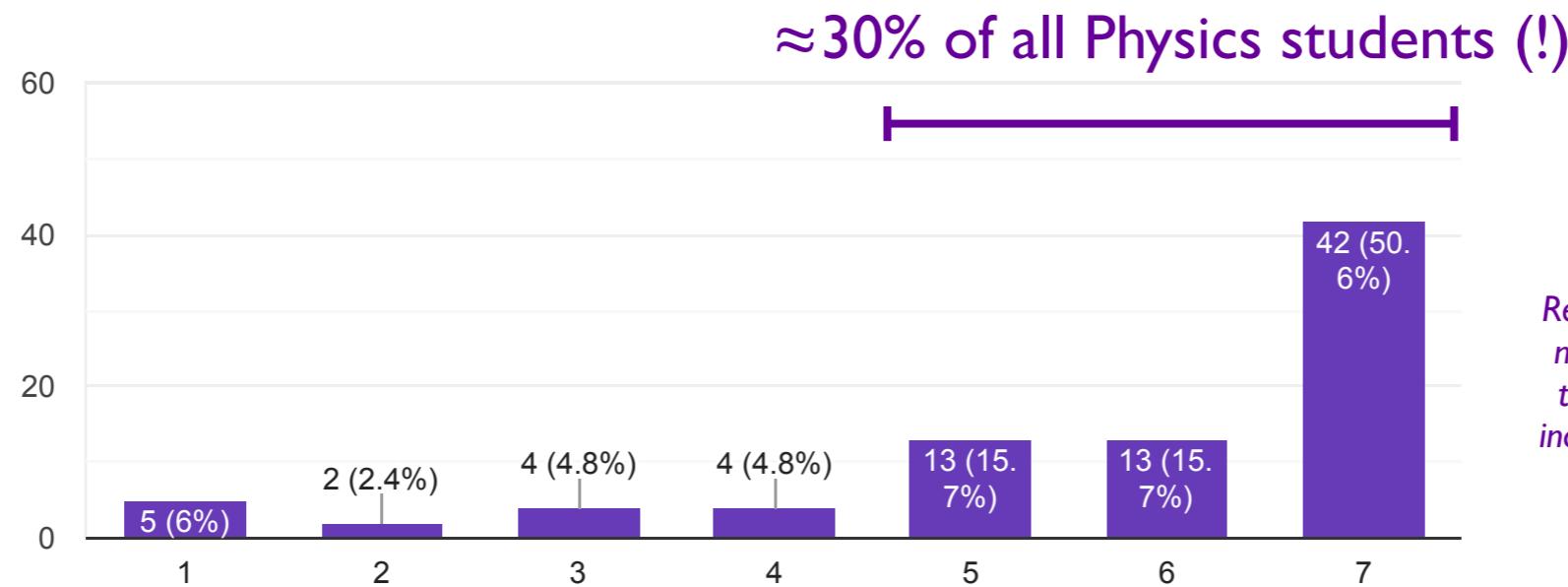


Interdisciplinary PhD in Physics, Statistics & Data Science



This interdisciplinary degree would have a number of requirements, in addition to the standard requirements for the MIT Physics PhD. How interested would you be in submitting and defending a PhD thesis that uses statistical methods in a substantial way?

83 responses



Respondent #11: "I think ML is the most important thing happening in the world right now and should be incorporated into any STEM degree."

*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*

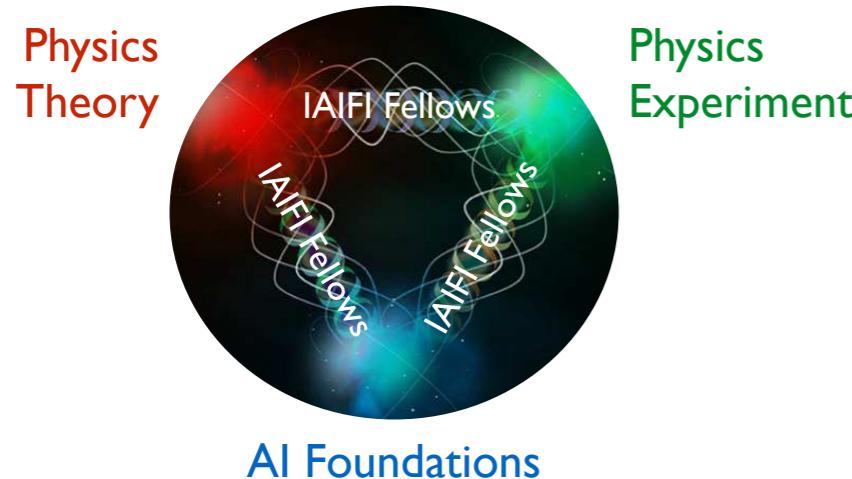
Programs like IAIFI Fellowships and Interdisciplinary PhD in Physics, Statistics & Data Science
offer unique opportunities for early-career researchers to pursue their interests

*IAIFI research has natural synergy with
the Schwarzman College of Computing*

“Machine Learning for the Physical Sciences” is growing dramatically, and
we envision possible new faculty hires in this area, e.g. as a future SCoC cluster

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*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



We look forward to **collaborations**
and synergies with AI+D!

<http://iaifi.org/>