Collision Course

Artificial Intelligence meets Fundamental Interactions

Jesse Thaler

IAIFI Director

IDEaS AI Seminar, Georgia Tech — November 20, 2020

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

[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

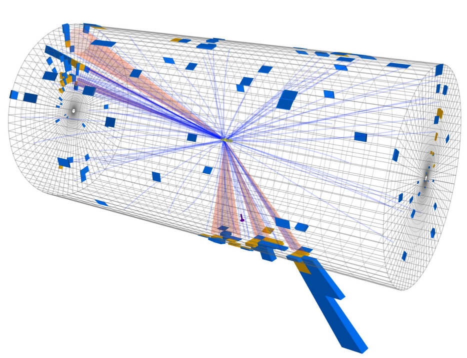
Physics Theory

Physics Experiment

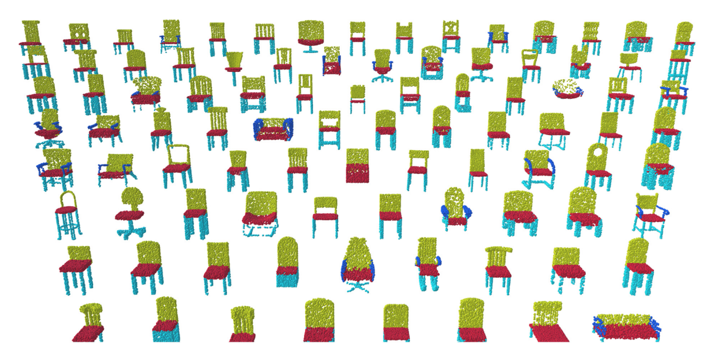
AI Foundations

- 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



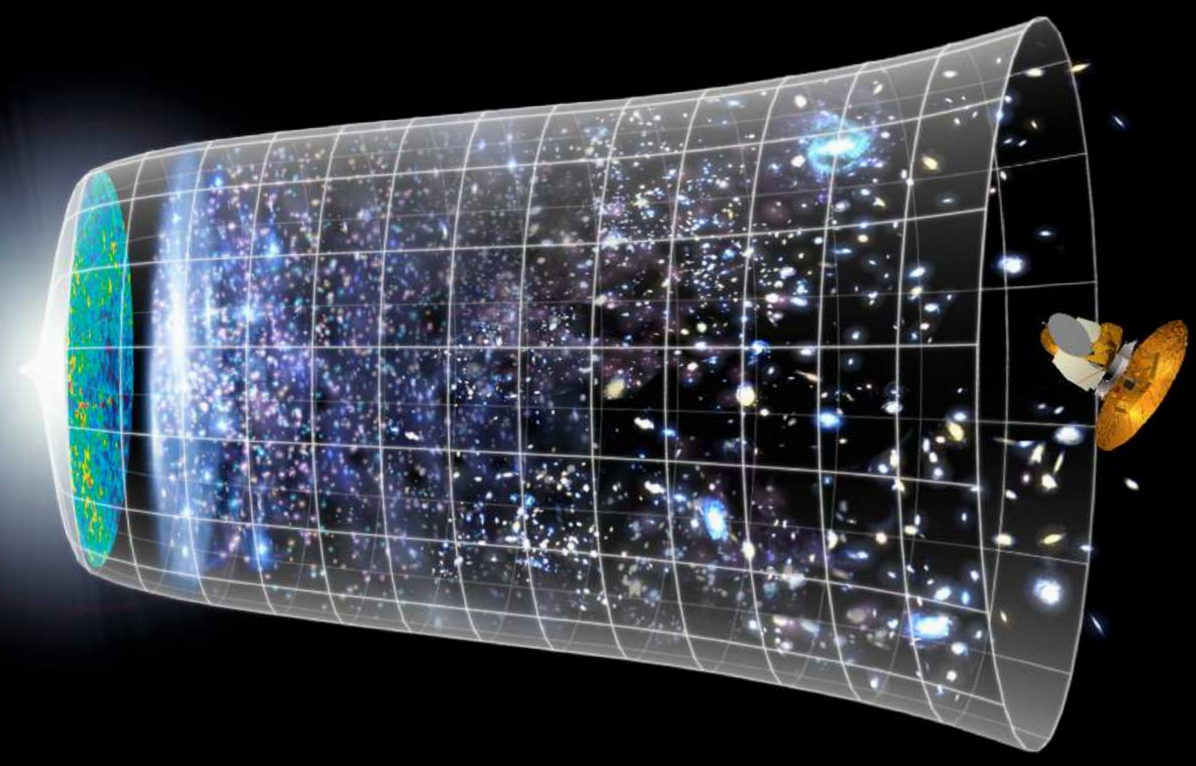
[Harris, Schwartz, JDT, Williams]



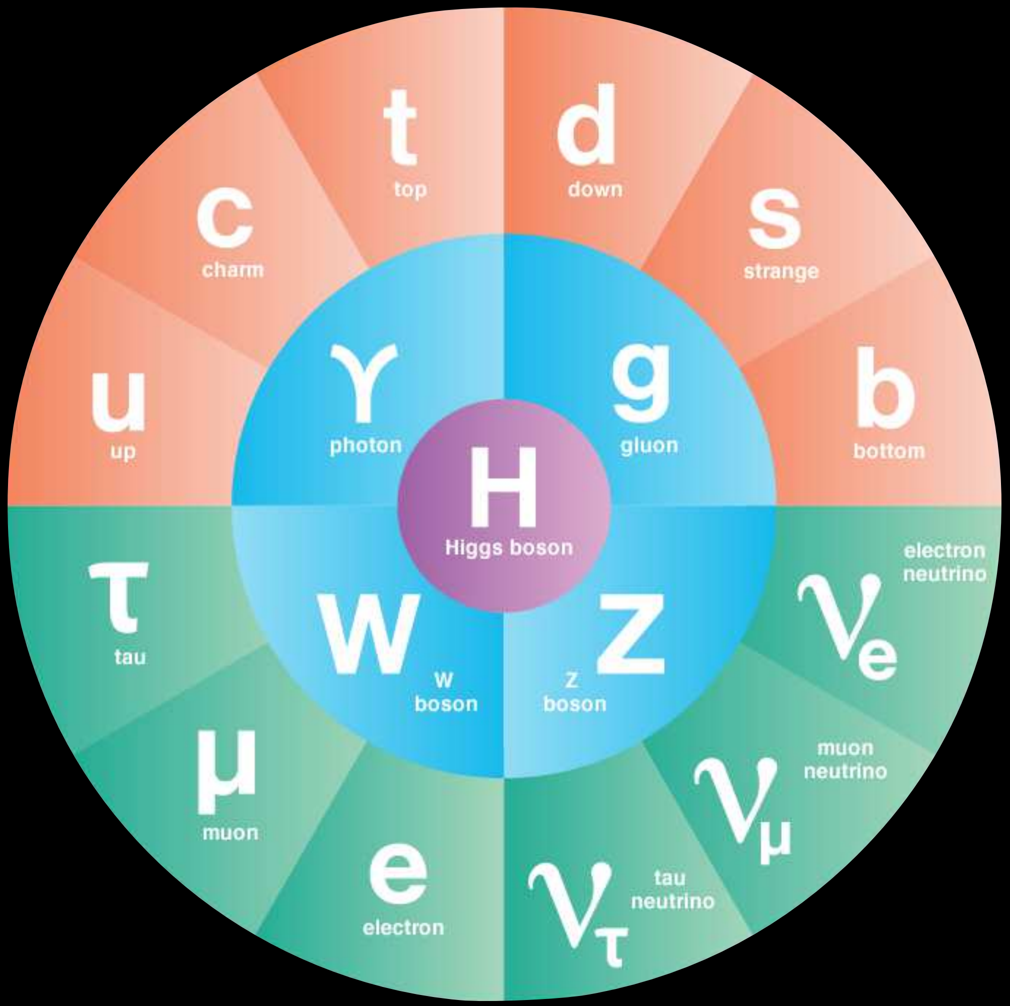
[Wang, Sun, Liu, Sarma, Bronstein, Solomon, TOG 2019]

Pillars of Fundamental Physics

Big Bang Cosmology



Standard Model

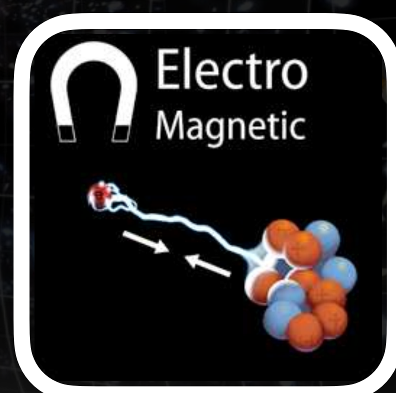


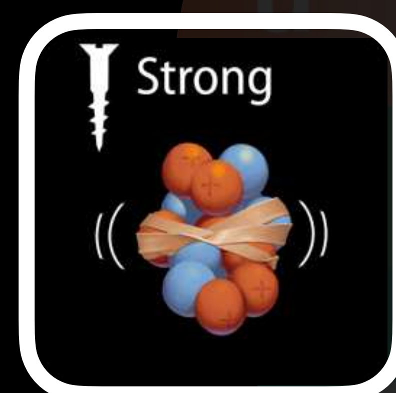
Pillars of Fundamental Physics

Big Bang Cosmology

Standard Model

Triumphs of Human Intelligence

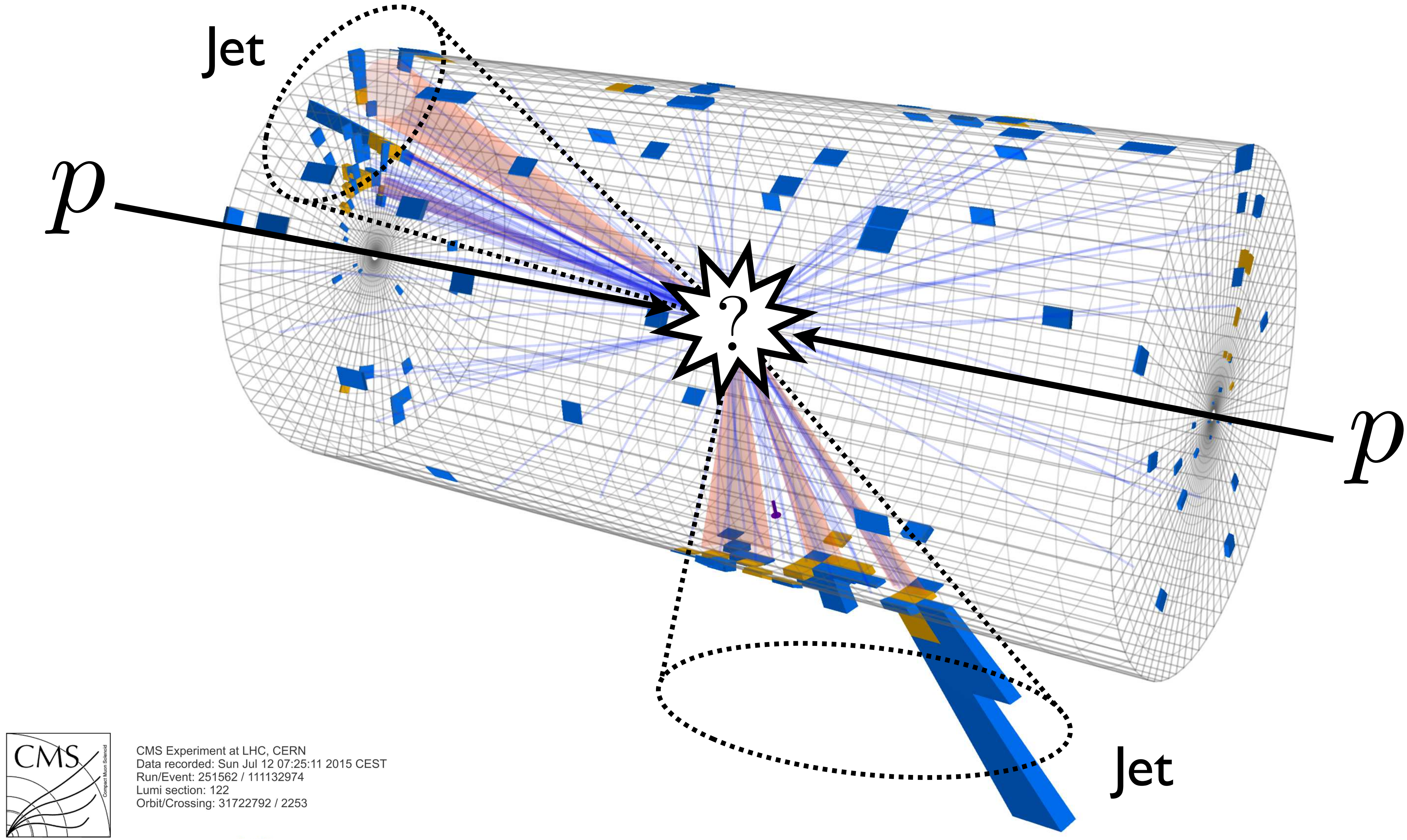




My research focus

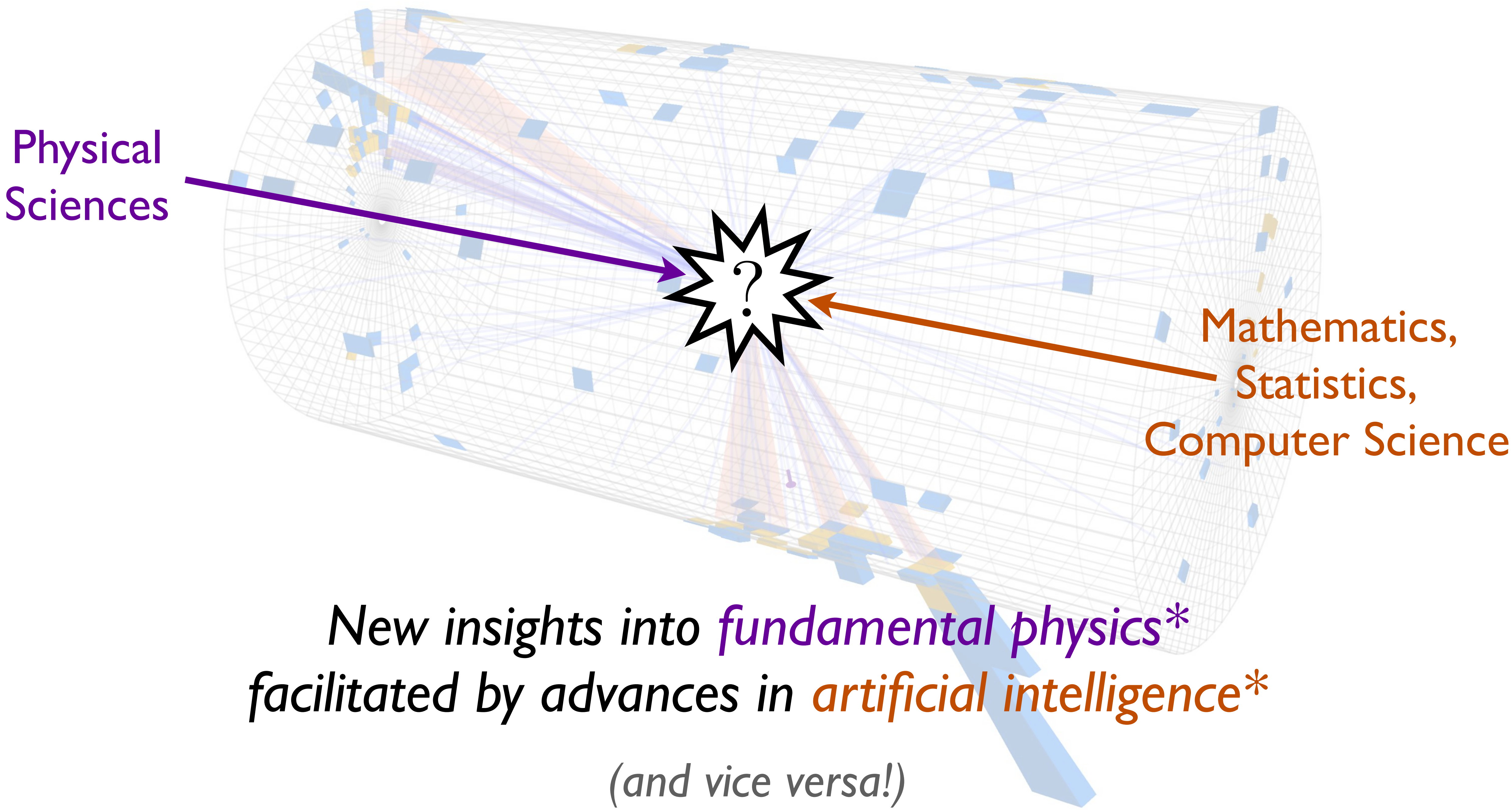
“Collision Course”

“[Theoretical Physics for Machine Learning](#)”
Aspen Center for Physics, January 2019



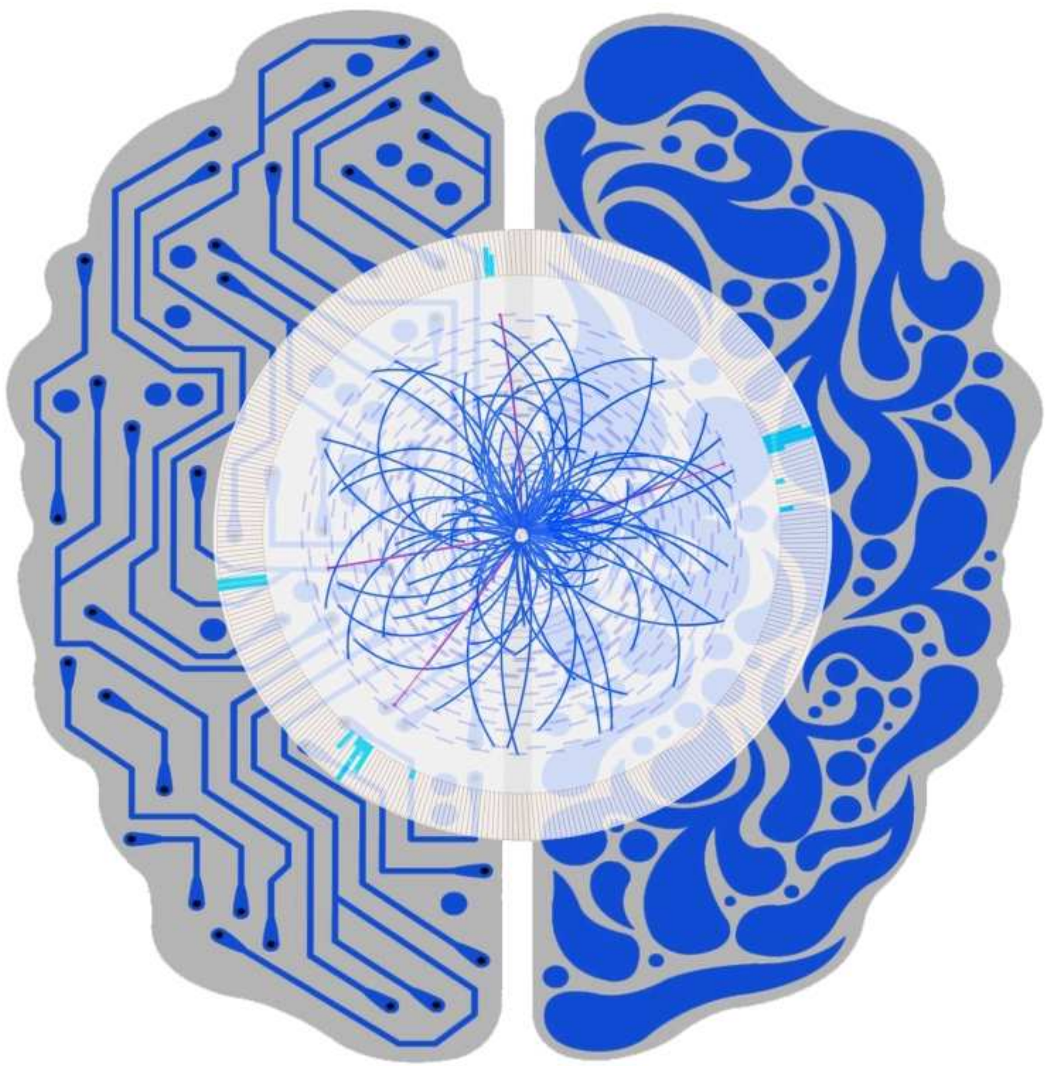
“Collision Course”

“Theoretical Physics for Machine Learning”
Aspen Center for Physics, January 2019



*New insights into fundamental physics**
*facilitated by advances in artificial intelligence**

(and vice versa!)



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

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

Deep Learning

E.g. Inpainting

Corrupted

Deep Image Prior

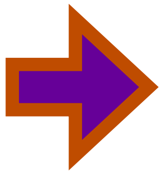
increased computational power and large data sets

[Ulyanov, Vedaldi, Lempitsky, CVPR 2018]

Deep Learning meets Deep Thinking

E.g. Inpainting

Corrupted



Deep Image Prior

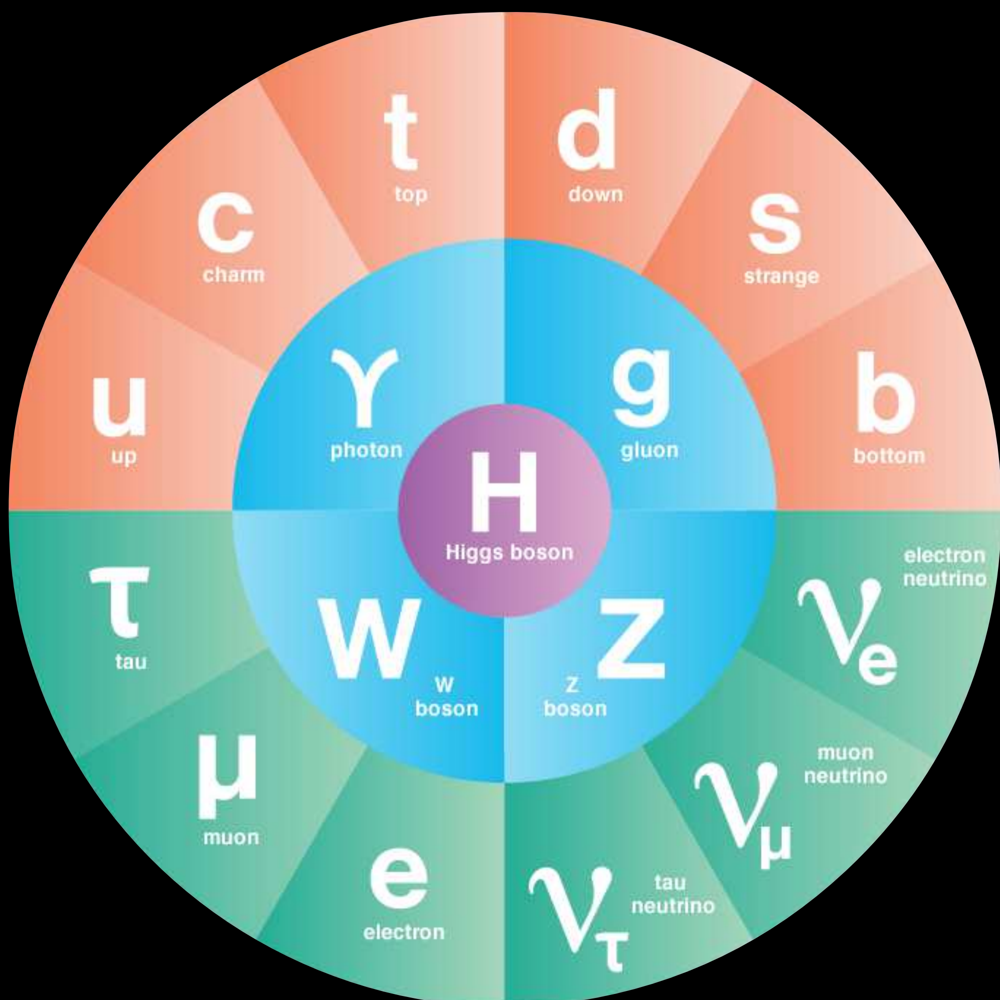
Using randomly initialized neural network (!)

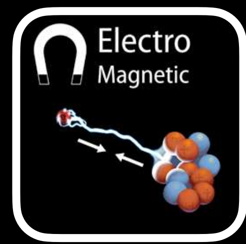
Progress made by understanding the structure of problems

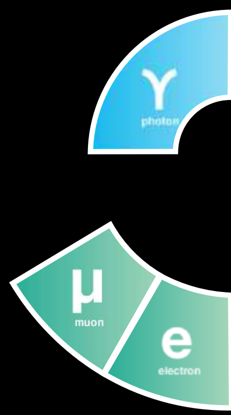
(not just increased computational power and large data sets)

[Ulyanov, Vedaldi, Lempitsky, CVPR 2018]

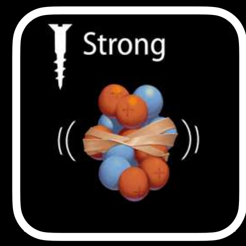
Particle Physics 101

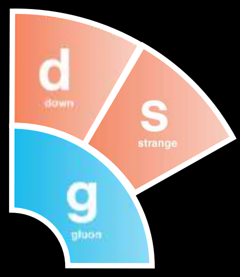






Quarks
&
Gluons





elementary

γ photon

$e^{\pm}$ electron

$\mu^{\pm}$ muon

composite

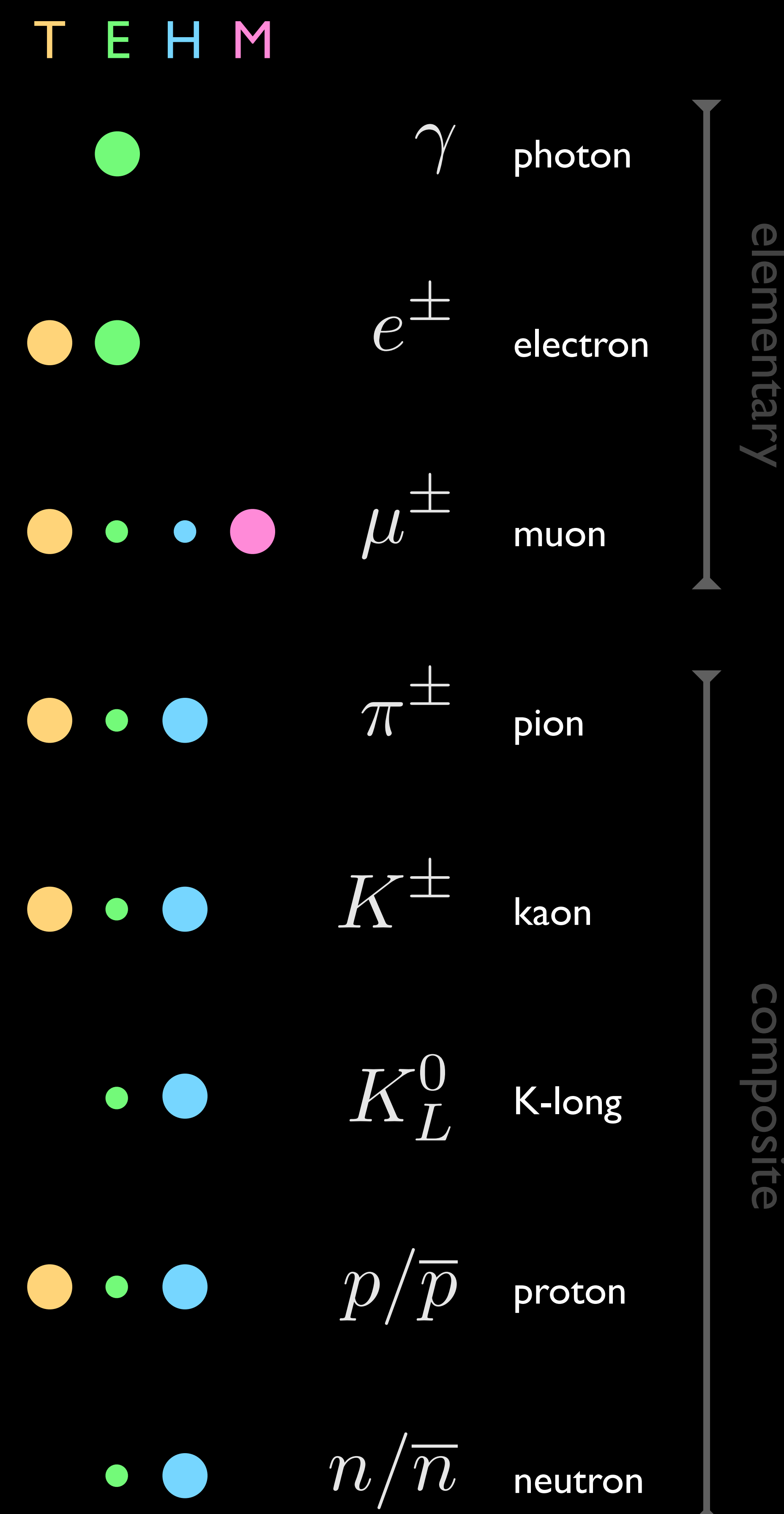
$\pi^{\pm}$ pion

$K^{\pm}$ kaon

K^0_L K-long

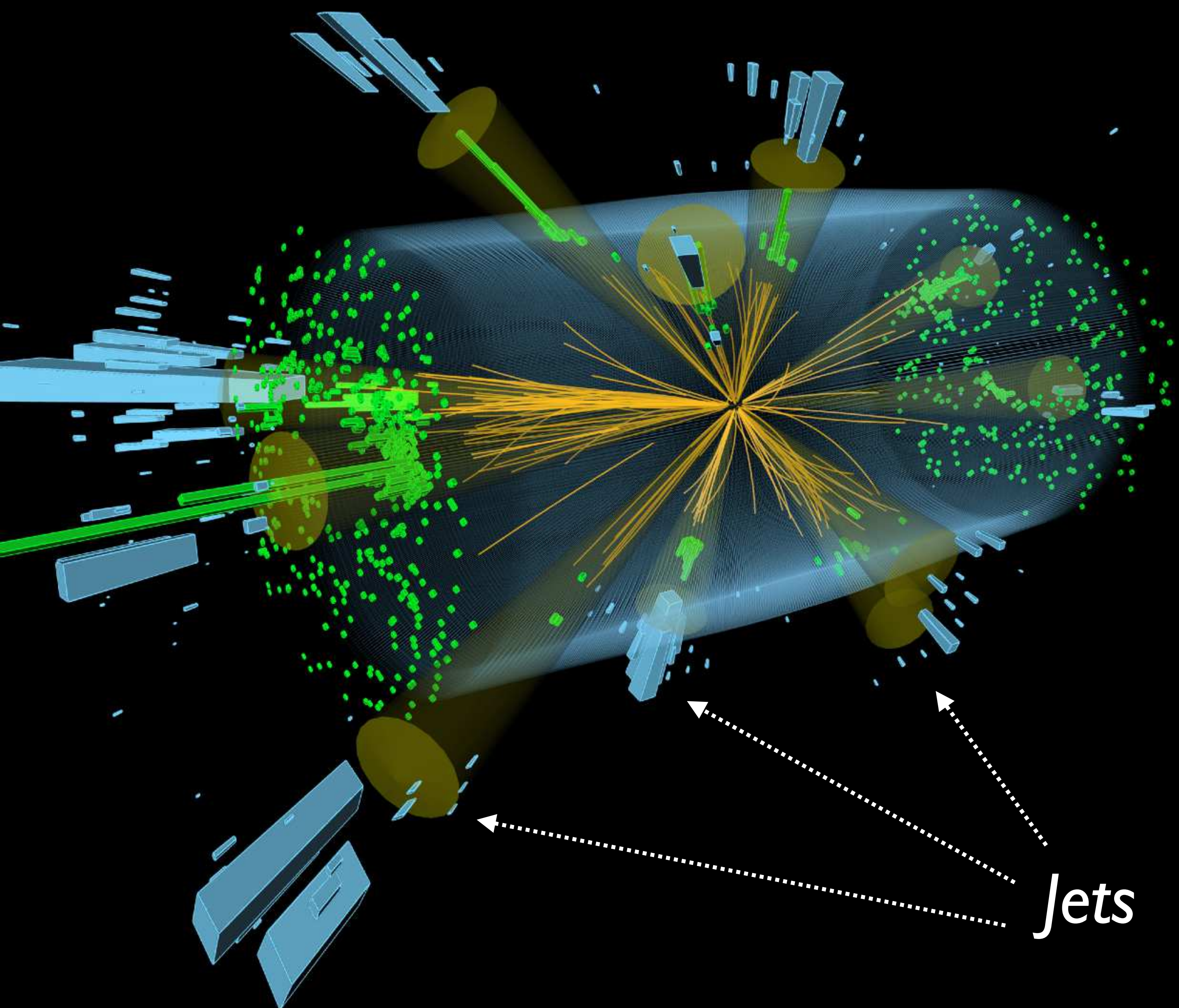
$p/\overline{p}$ proton

$n/\overline{n}$ neutron


T E H M
γ photon
$e^{\pm}$ electron
$\mu^{\pm}$ muon
$\pi^{\pm}$ pion
$K^{\pm}$ kaon
K_L^0 K-long
$p/\overline{p}$ proton
$n/\overline{n}$ neutron
elementary
composite

Collider Event

Collection of points in (momentum) space



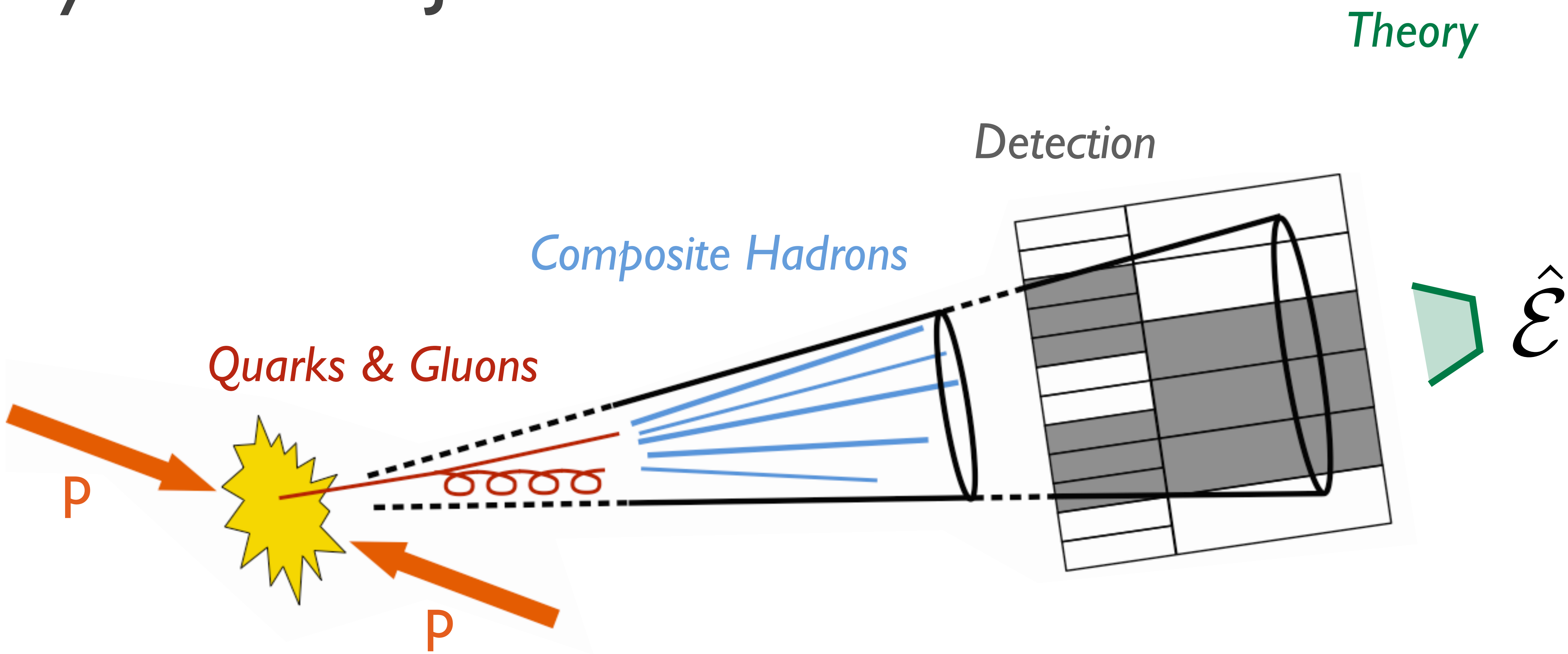
	T	E	H	M		
elementary		●			γ	photon
	●	●			$e^{\pm}$	electron
	●	●	●	●	$\mu^{\pm}$	muon
composite	●	●	●		$\pi^{\pm}$	pion
	●	●	●		$K^{\pm}$	kaon
		●	●		K_L^0	K-long
	●	●	●		$p/\overline{p}$	proton
		●	●		$n/\overline{n}$	neutron

Point Cloud

Collection of points in (position) space

[Popular Science, 2013]

Dynamics of Jet Formation



Energy Flow:

Robust to hadronization and detector effects

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

[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, PRD 2020]

Patrick Komiske

Eric Metodiev

Principles of Fundamental Physics

Robustness of Energy Flow

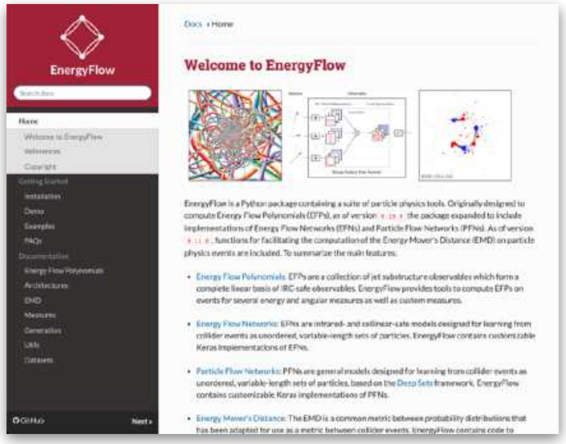
[Komiske, Metodiev, JDT, JHEP 2018]

?

Power of Artificial Intelligence

Point Cloud Learning

[Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, NIPS 2017]



Energy Flow Networks

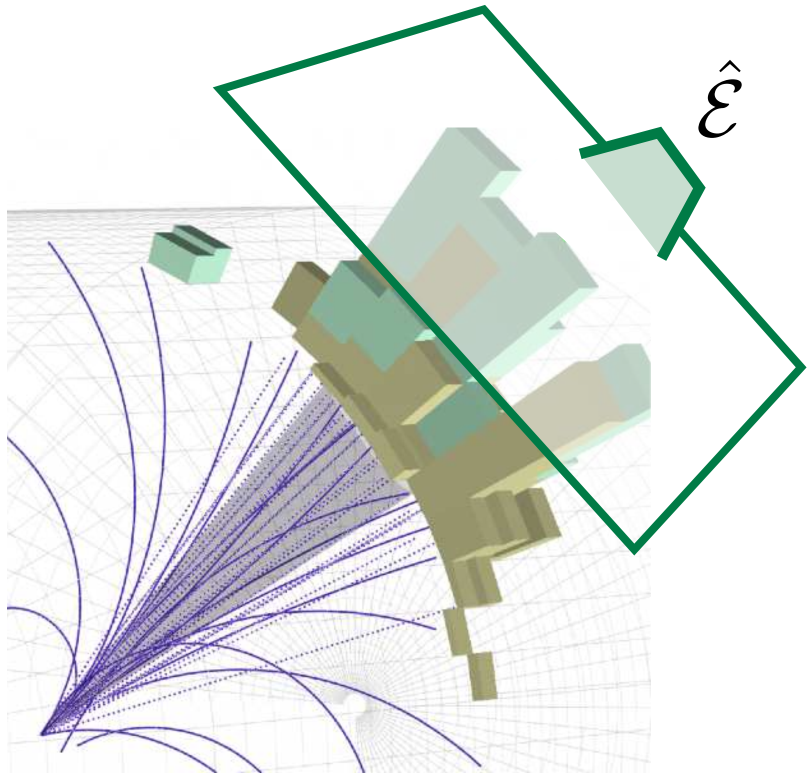
https://energyflow.network/
[Komiske, Metodiev, JDT, JHEP 2019]

Jets as Weighted Point Clouds

- Energy-Weighted Directions

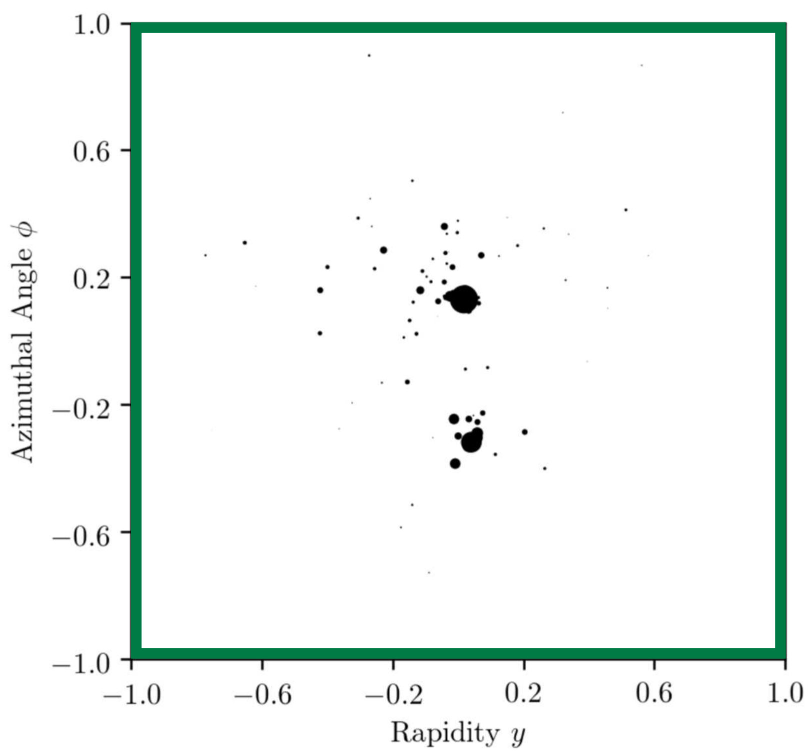
$$\vec{p} = \{\underbrace{E}_{\text{Energy}}, \underbrace{\hat{n}_x, \hat{n}_y, \hat{n}_z}_{\text{Direction}}\}$$

(suppressing "unsafe" charge/flavor information)



- Equivalently: Energy Density

$$\rho(\hat{n}) = \sum_{i \in \mathcal{J}} \underbrace{E_i}_{\text{Energy}} \, \delta^{(2)}(\hat{n} - \underbrace{\hat{n}_i}_{\text{Direction}})$$



"Thinking" Like a Physicist

Symmetry: $\mathcal{J} = \{\underbrace{\vec{p}_1, \vec{p}_2, \vec{p}_3, \ldots, \vec{p}_N}_{\text{Unordered, Variable Length Set (QM!)}}\}$

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

Energy weighting (QFT!)

Properly specified problem

Many (labeled) examples $\{\mathcal{J}\}$

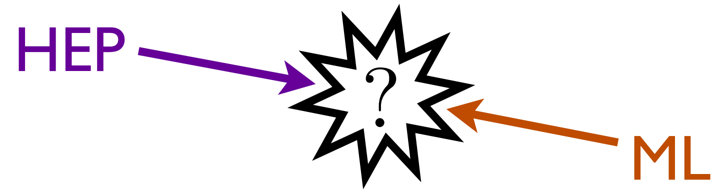
The Machine

Solution $S(\mathcal{J})$

Verification $V(\mathcal{J})$

Check that answer is physically sensible

Energy Flow Networks



Architecture designed around symmetries and interpretability

Permutation invariant

Linear weights (i.e. safe)

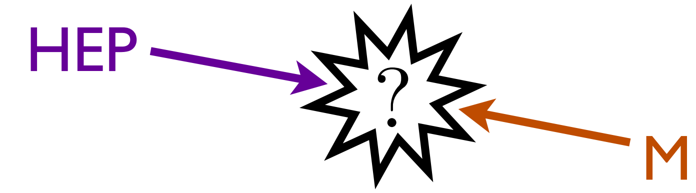
$$S(\mathcal{J}) = F(V_1, V_2, \ldots, V_\ell) \qquad V_a(\mathcal{J}) = \sum_{i \in \mathcal{J}} E_i \, \Phi_a(\hat{n}_i)$$

Parametrized with Neural Networks

Provably describes any safe observable (!)*
Excellent jet classification performance

[Komiske, Metodiev, JDT, JHEP 2019; see also Komiske, Metodiev, JDT, JHEP 2018; code at energyflow.network; special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, NIPS 2017]

Energy Flow Networks



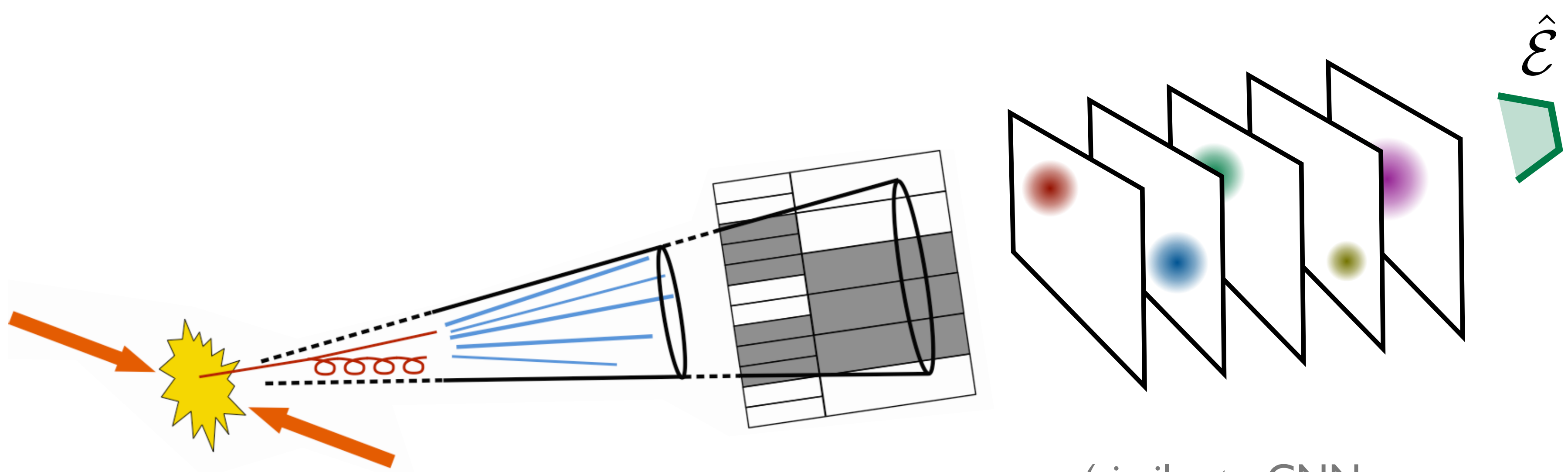
Architecture designed around symmetries and interpretability

Latent space of dim ℓ

$$S(\mathcal{J}) = F\left(V_1, V_2, \ldots, V_\ell\right) \qquad V_a(\mathcal{J}) = \sum_{i \in \mathcal{J}} E_i \, \Phi_a(\hat{n}_i)$$

Can visualize if ℓ is small

Easy to plot!

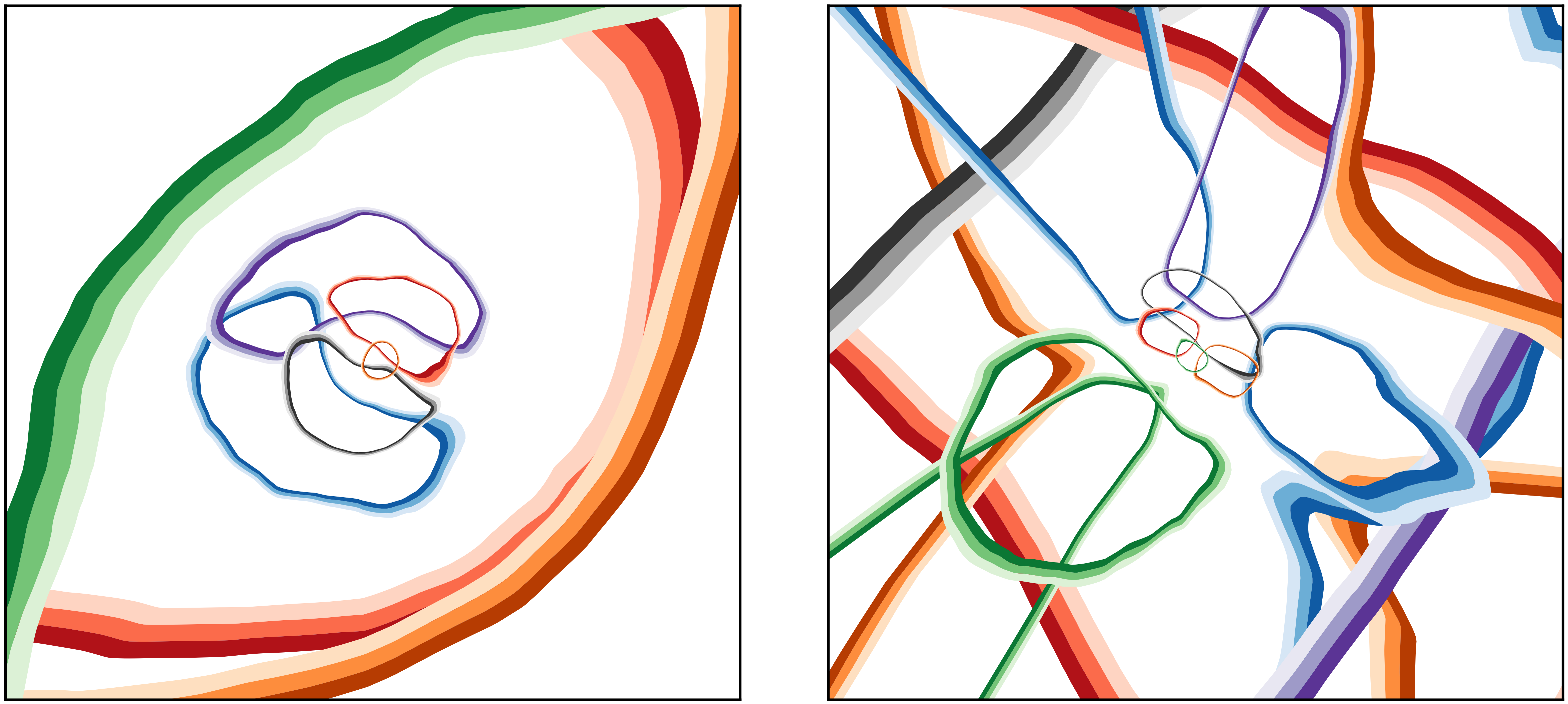


(similar to CNN filter activation)

[Komiske, Metodiev, JDT, JHEP 2019; see also Komiske, Metodiev, JDT, JHEP 2018; code at energyflow.network; special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, NIPS 2017]

Psychedelic Network Visualization

Latent Dimension 8 | Latent Dimension 16

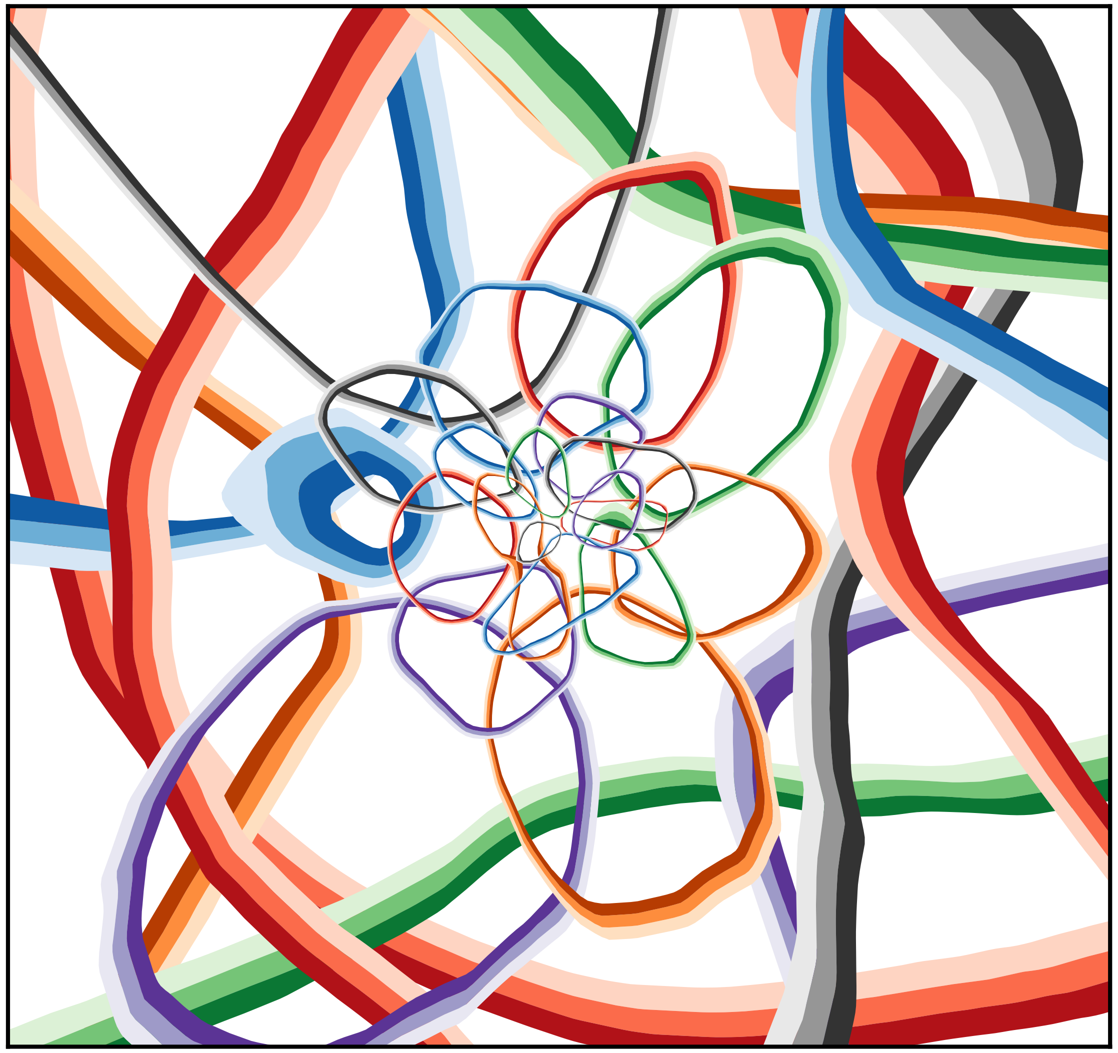


"Hello, World!" of Jets: Quark 

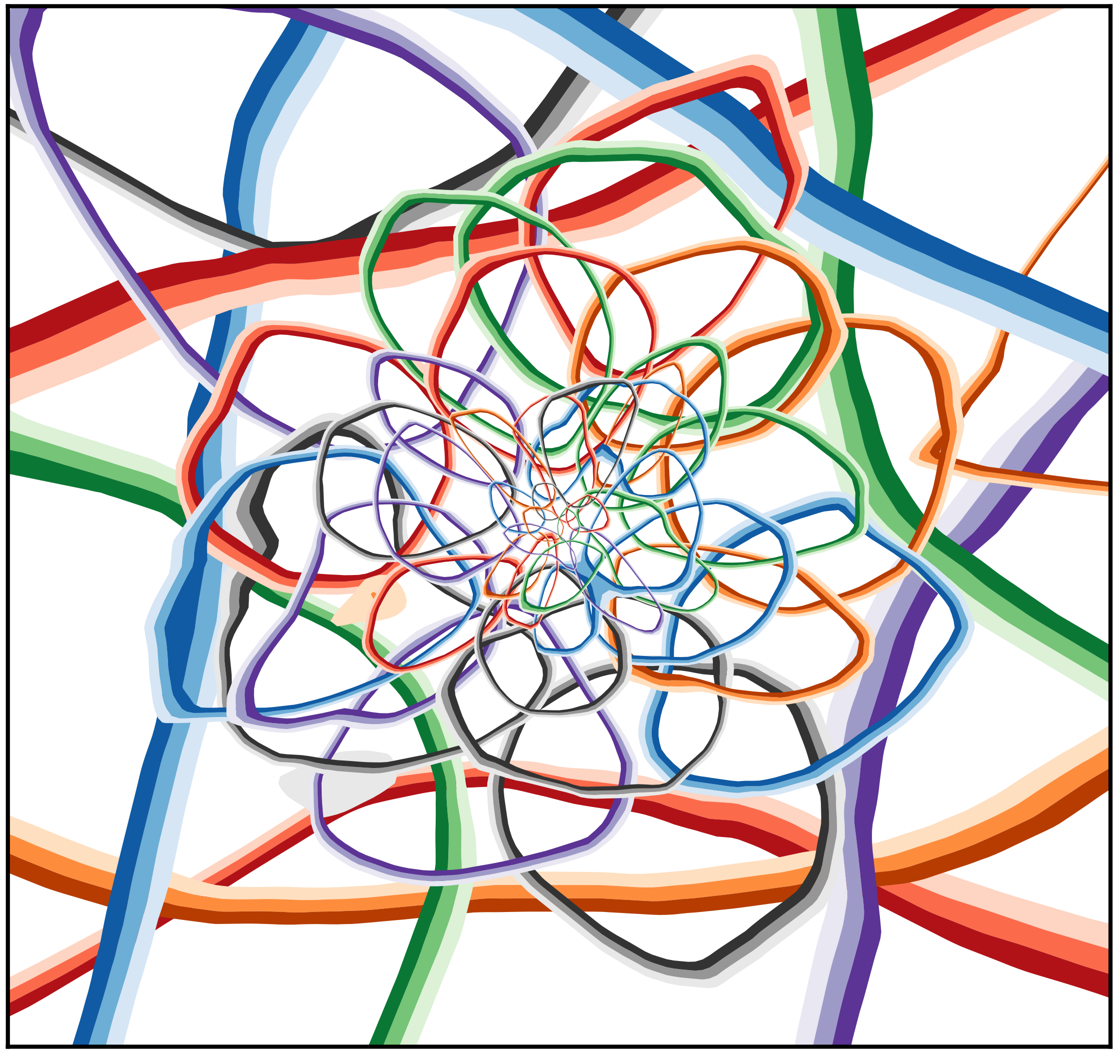
vs. Gluon 

Psychedelic Network Visualization

Latent Dimension 32

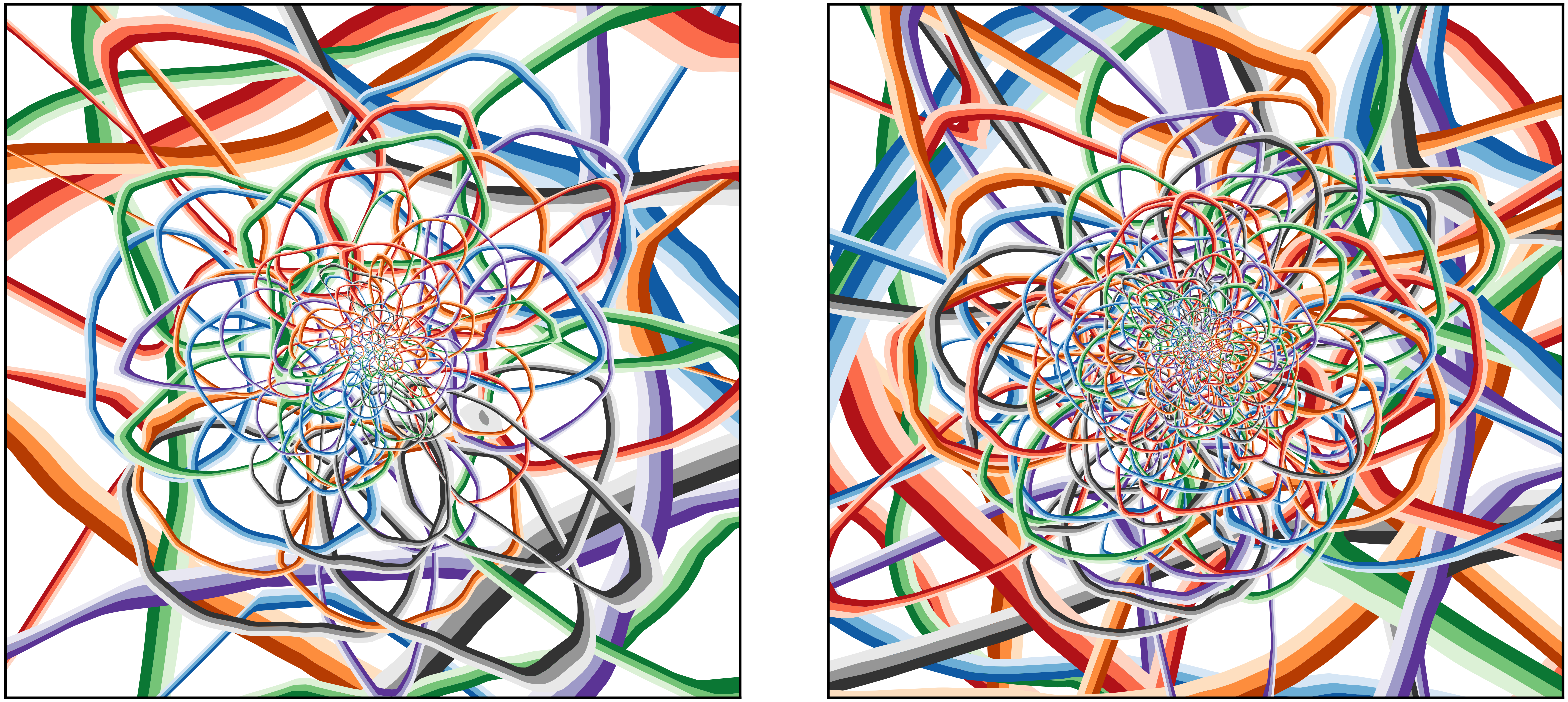


Latent Dimension 64



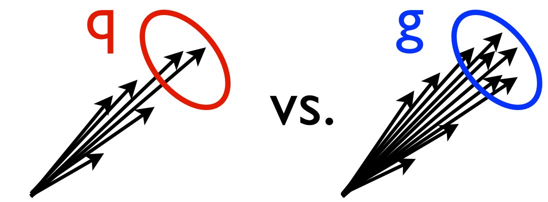
Psychedelic Network Visualization

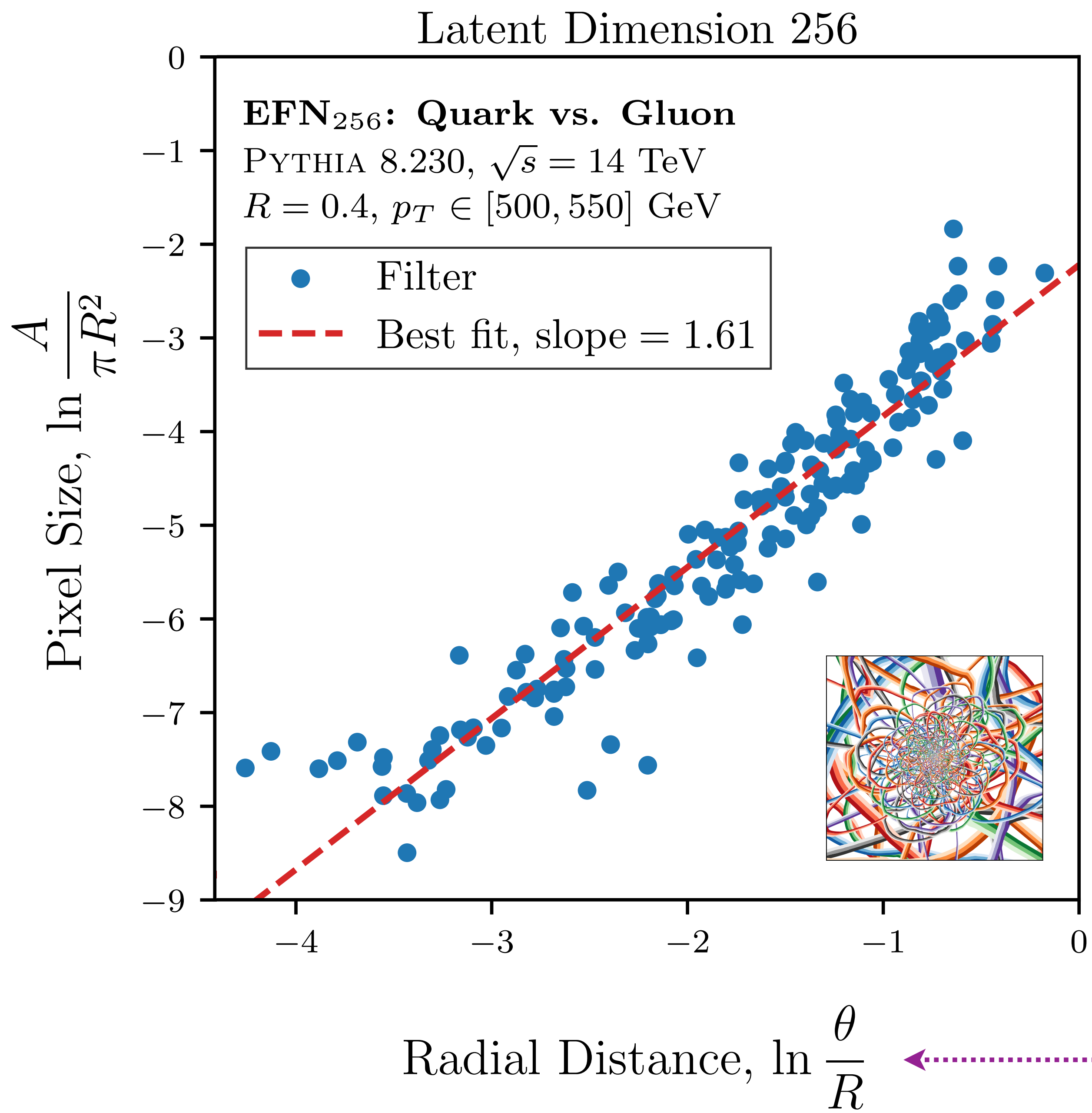
Latent Dimension 128 | Latent Dimension 256

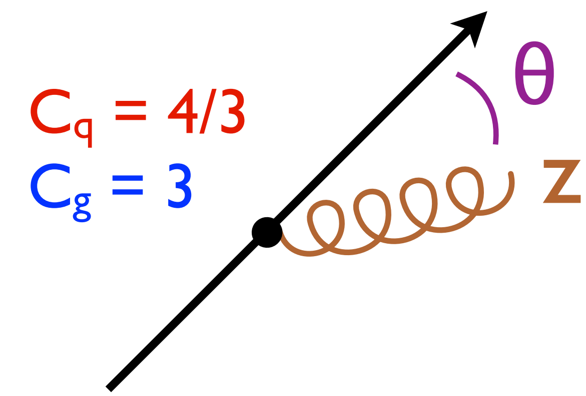


Fractal structure of the strong force!

Scaling of Strong Interactions



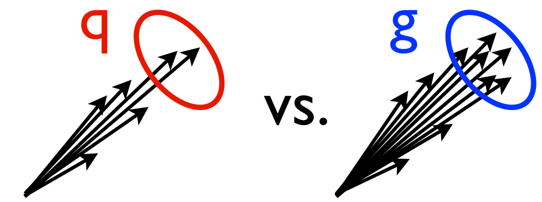




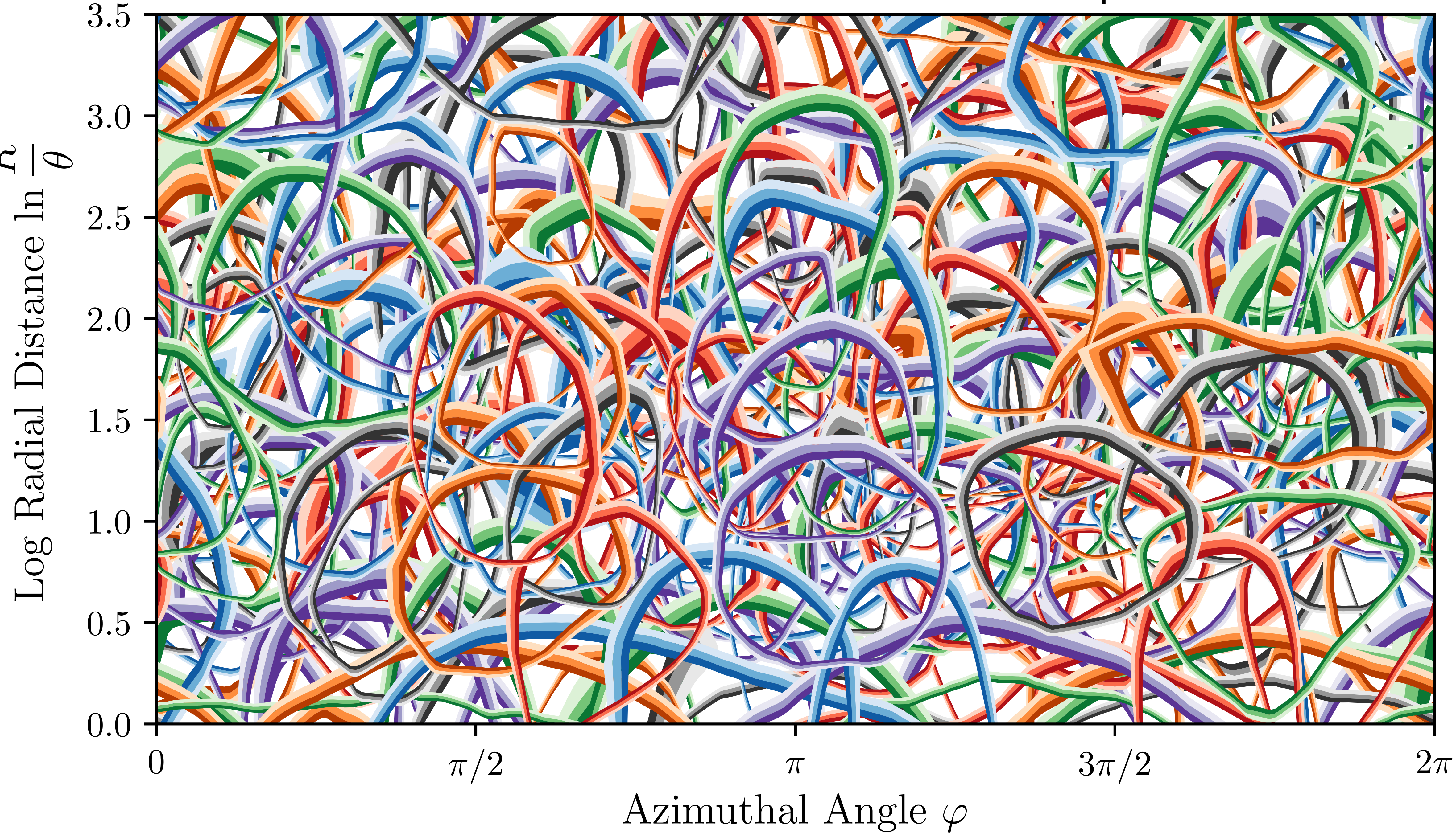
$$\mathrm{d}P_{i \to ig} \simeq \frac{2\alpha_s}{\pi} C_i \underbrace{\frac{\mathrm{d}\theta}{\theta}}_{\text{Collinear}} \underbrace{\frac{\mathrm{d}z}{z}}_{\text{Soft}}$$

[Komiske, Metodiev, JDT, JHEP 2019]

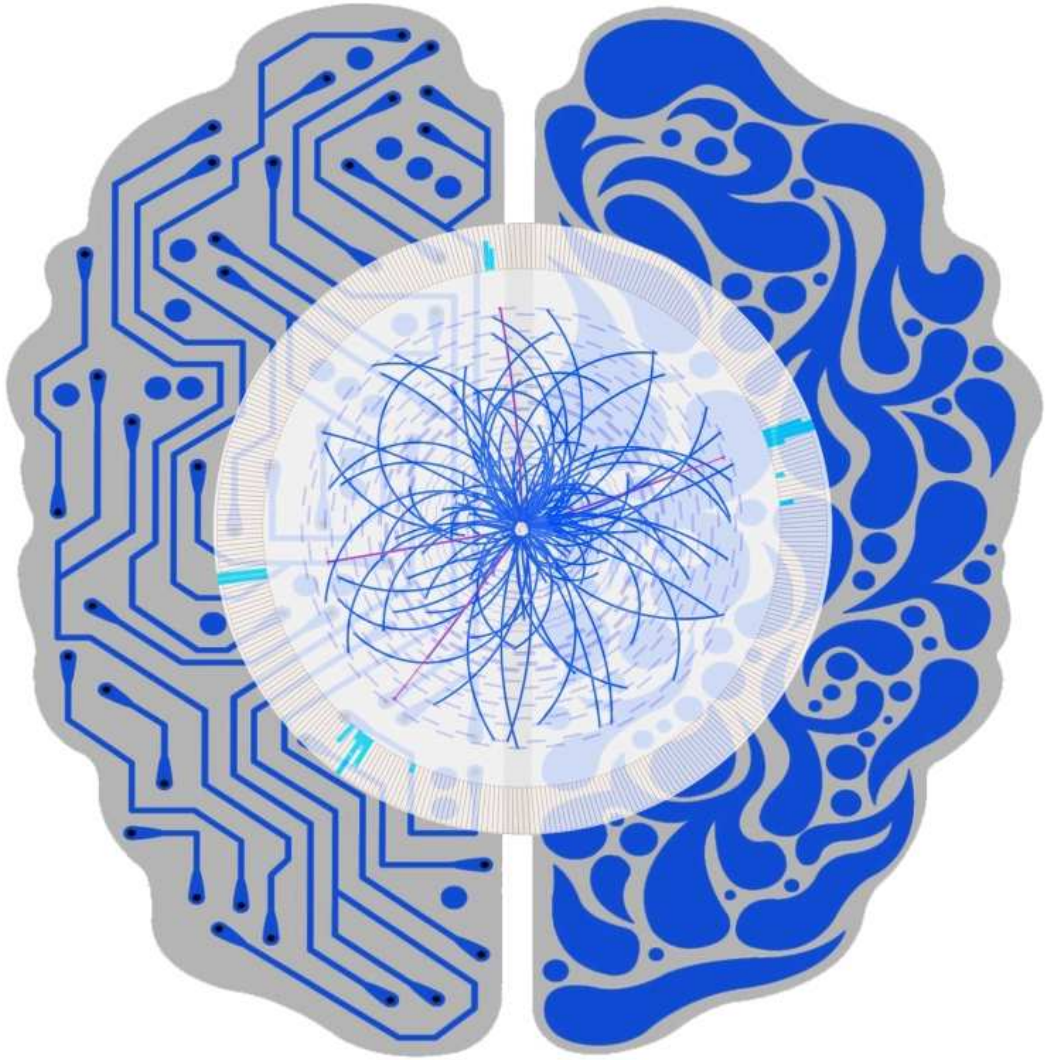
Ready for the High Museum?



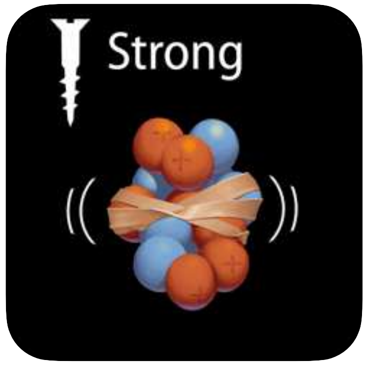
Coordinate transformation to the emission plane



[Komiske, Metodiev, JDT, JHEP 2019; see also Dreyer, Salam, Soyez, JHEP 2018]



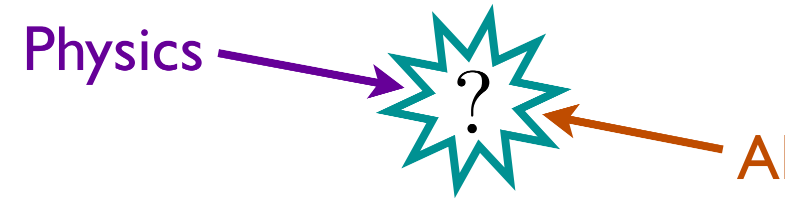
We taught a machine to "think" like a physicist…



…and it learned fractal structure of strong force!

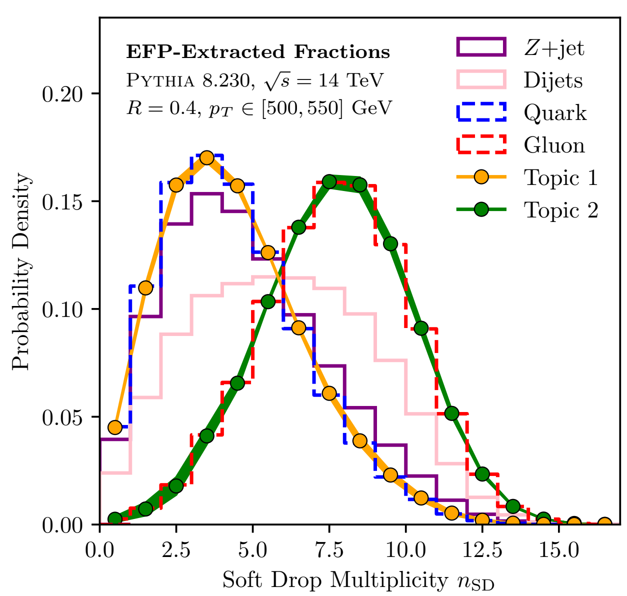
(see backup for something new it taught us)

“Collision Course”



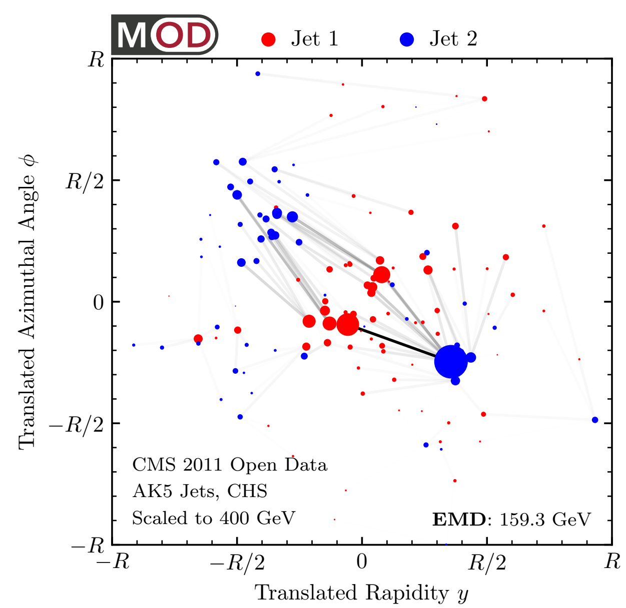
New insights into fundamental physics facilitated by advances in mathematics, statistics, and computer science (and vice versa!)

Quark/Gluon Definitions via Blind Source Separation



[Metodiev, JDT, PRL 2018; Komiske, Metodiev, JDT, JHEP 2018]

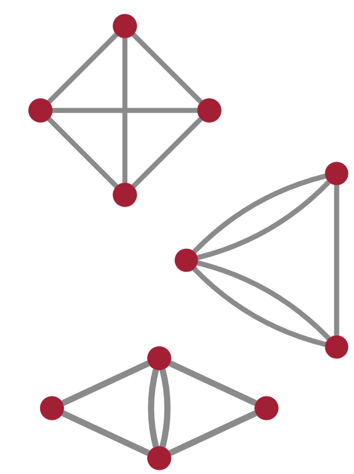
Half-Century of Collider Physics via Optimal Transport (!)



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

Kinematic Decomposition via Graph Theory

	Leafless Multigraphs	
	Connected	All
Edges d	A307317	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:

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

LNS rle AT MIT MIT CSAIL MIT KAVLI INSTITUTE IDSS MIT INSTITUTE FOR DATA, SYSTEMS, AND SOCIETY

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

Taritree Wongjirad

Boston Area: Critical Mass for Transformative Ab Initio AI Research

AI^2: Ab Initio Artificial Intelligence

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

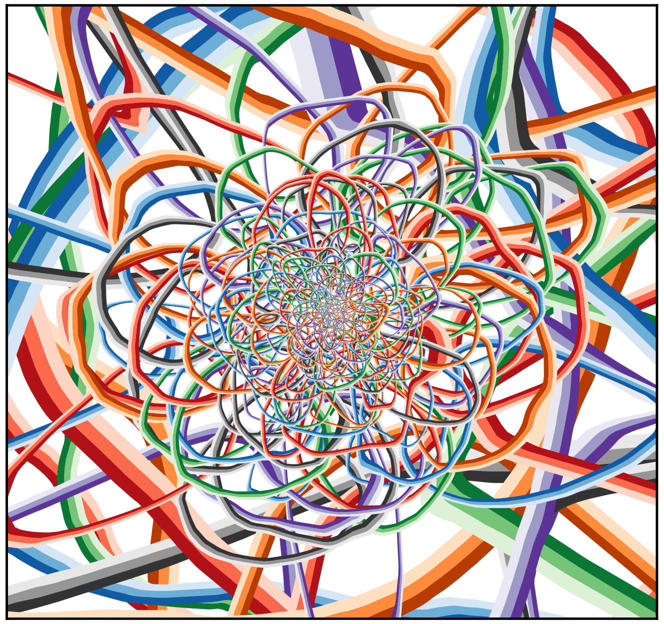
Symmetries, conservation laws, scaling relations, limiting behaviors, locality, causality,
unitarity, gauge invariance, entropy, least action, factorization, unit tests,
exactness, systematic uncertainties, reproducibility, verifiability, …

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]

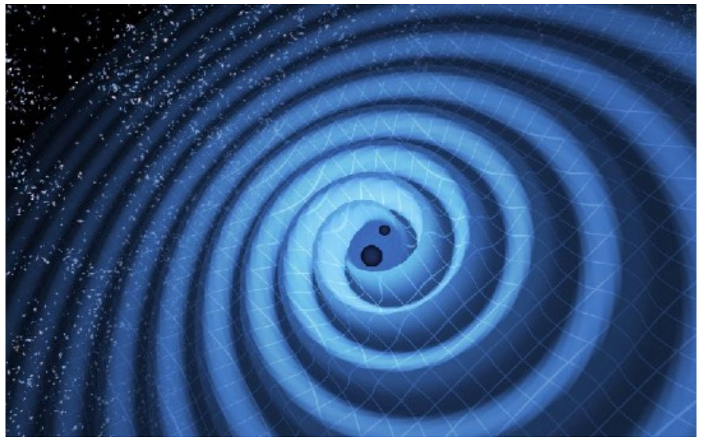
AI — Powerful strategy to analyze LHC collisions

× AI — Efficient neural network for point clouds

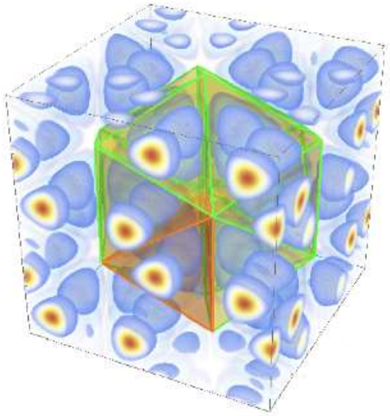
= AI² — Cross-cutting research across disciplines

Artificial Intelligence ⇔ *Fundamental Interactions*

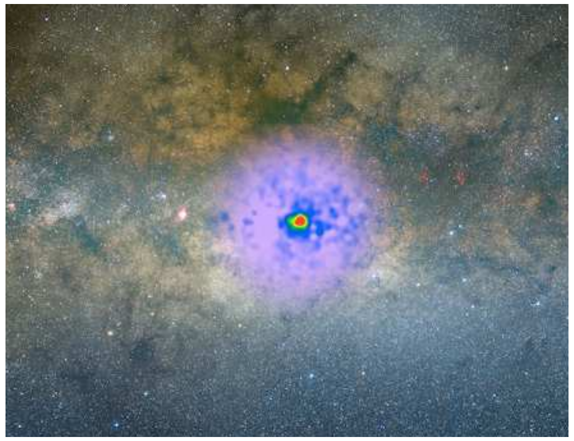
Gravitational Waves



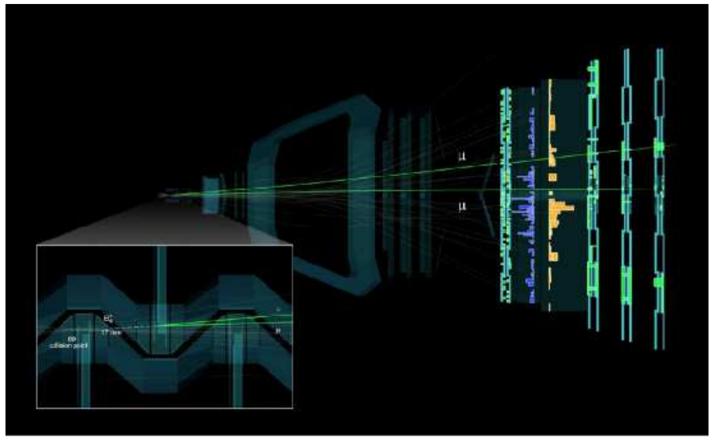
Nuclear Physics



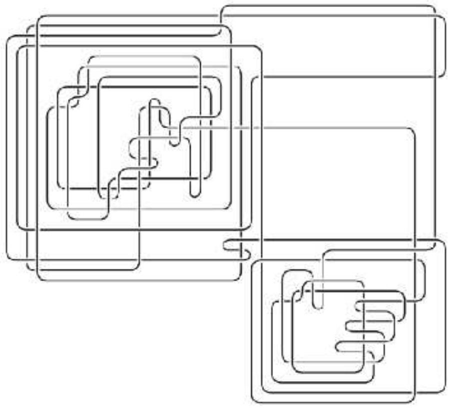
Astrophysics



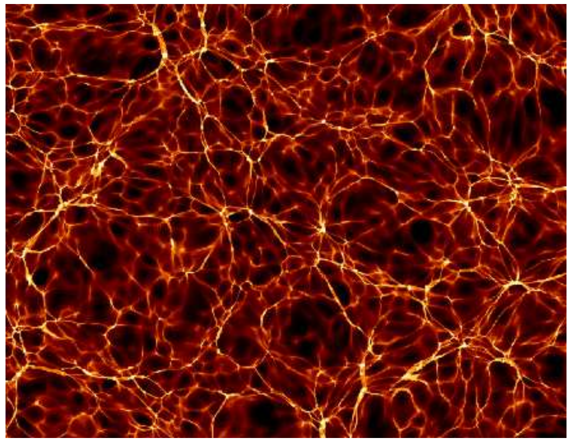
Particle Colliders



Mathematical Physics



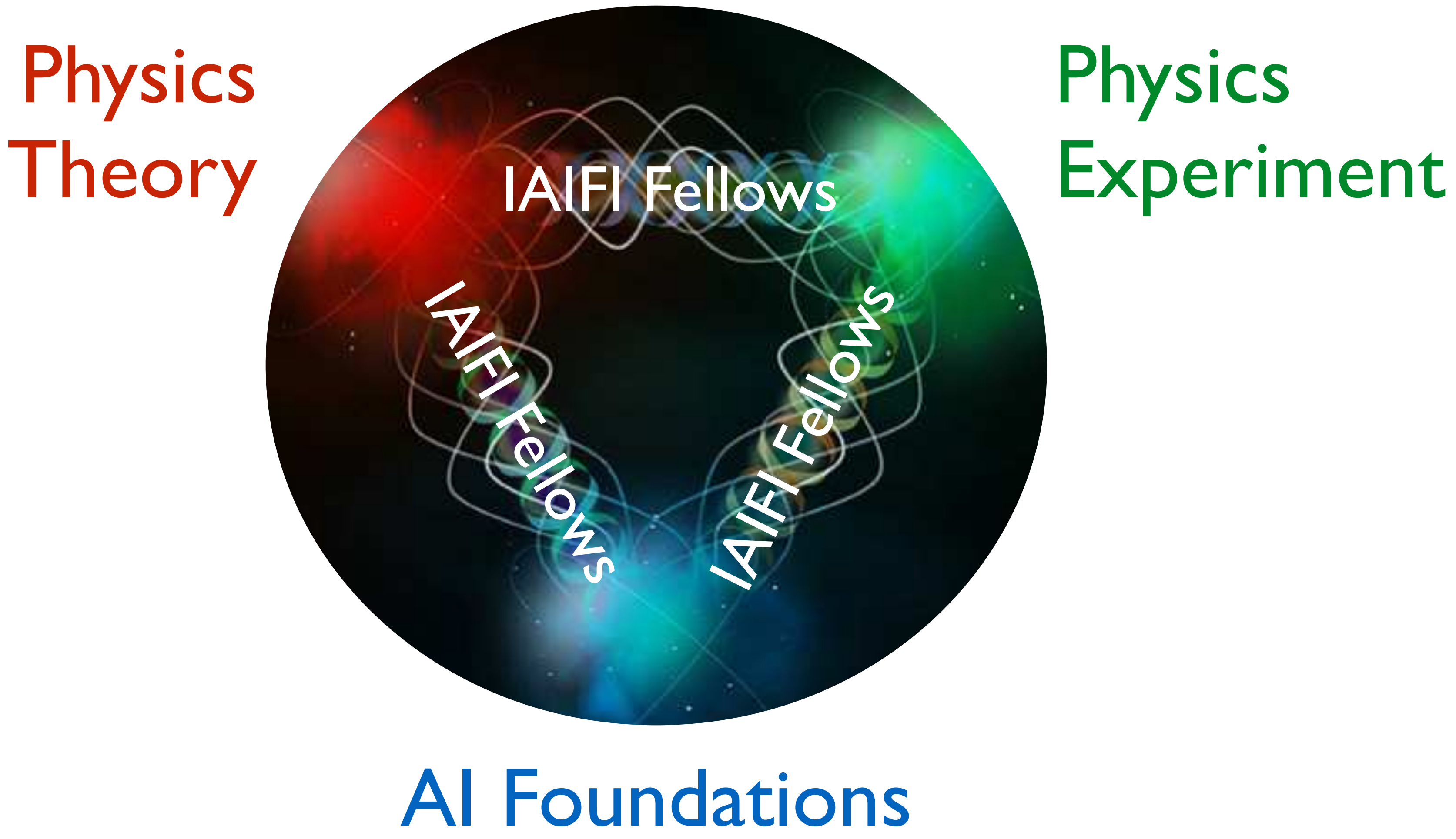
Dark Matter



…

IAIFI Postdoctoral Fellowships

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



[https://iaifi.org/fellows.html]

IAIFI Research Plan

Physics Theory

Physics Experiment

AI Foundations

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

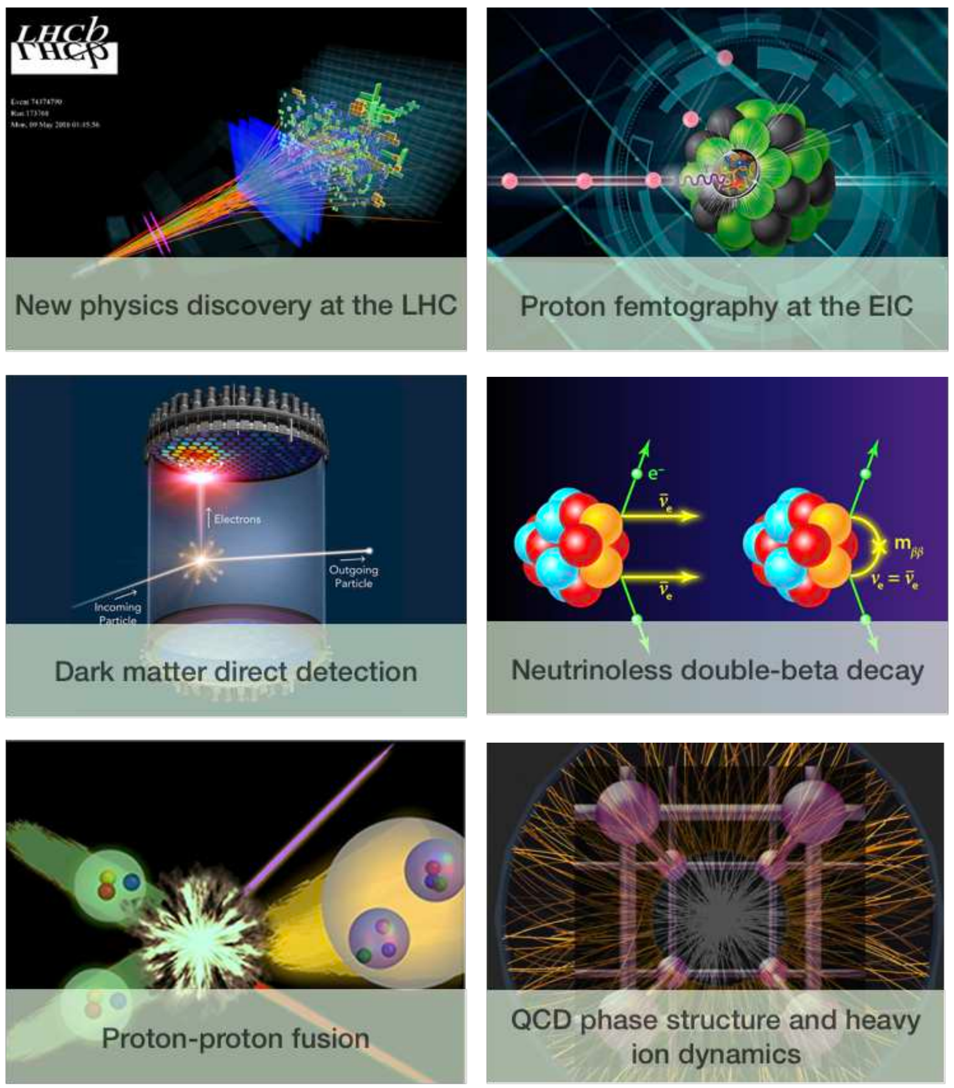
AI² for Foundational AI

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)



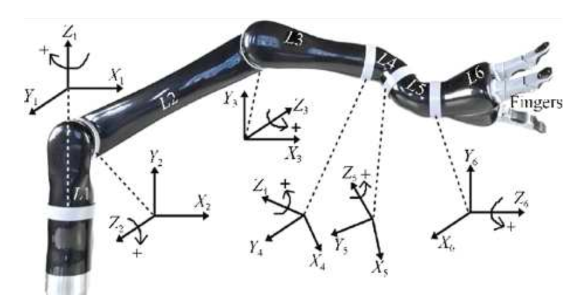
Industry collaboration to develop custom AI tools

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

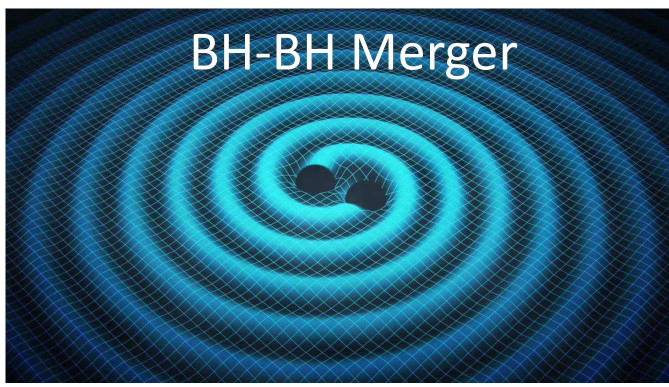


[Kanwar, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan, arXiv 2020]

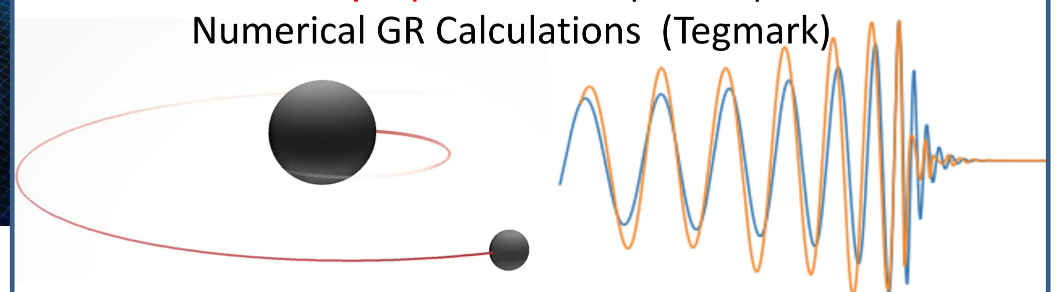
AI² for Experimental Physics

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

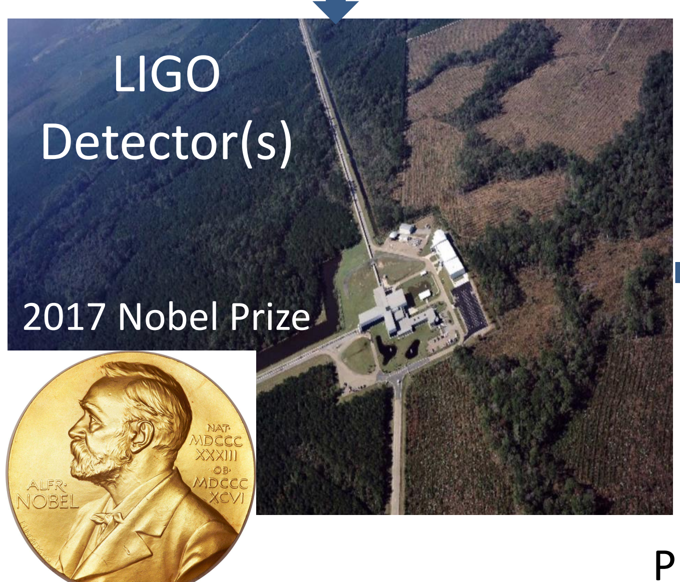


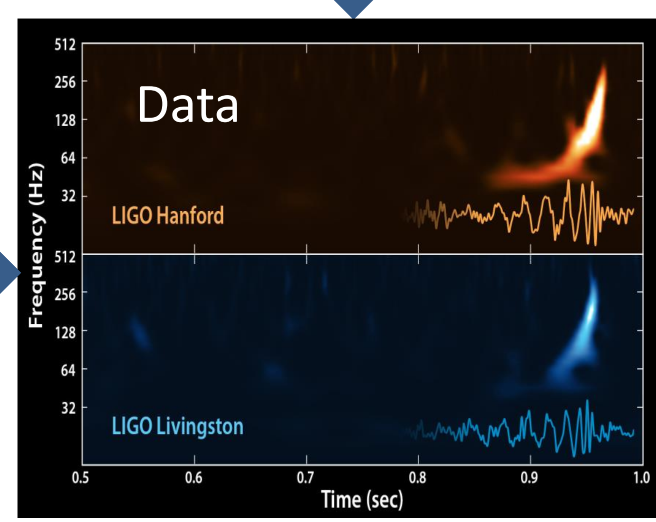
Theory Inputs: AI² to Speed Up Numerical GR Calculations (Tegmark)

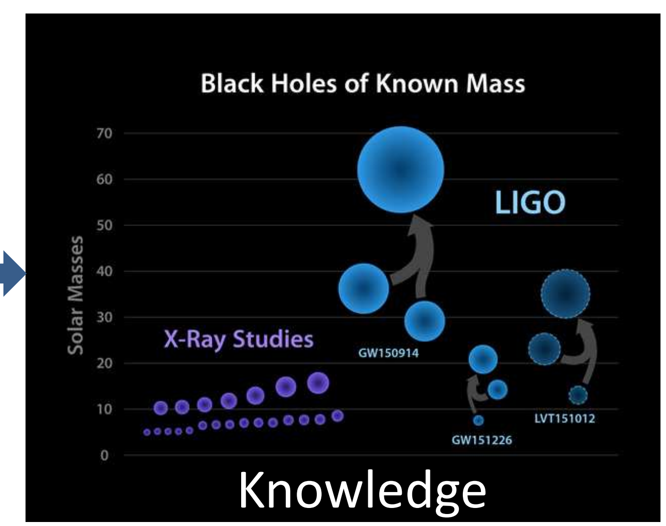


LHC Fast-ML to speed up multi-messenger astrophysics (Harris)

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







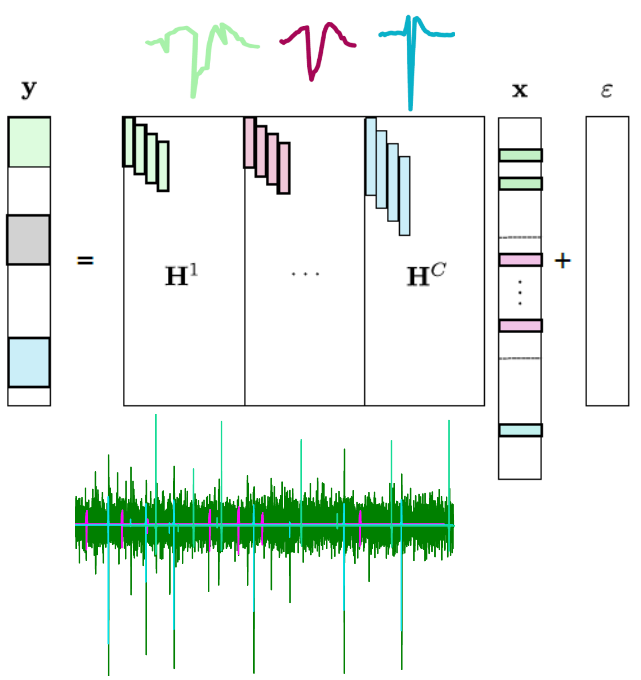
Propose using RL for Noise Reduction (Barsotti, Rakhlin)

AI² for Foundational AI

E.g. Deconvolution Across Disciplines

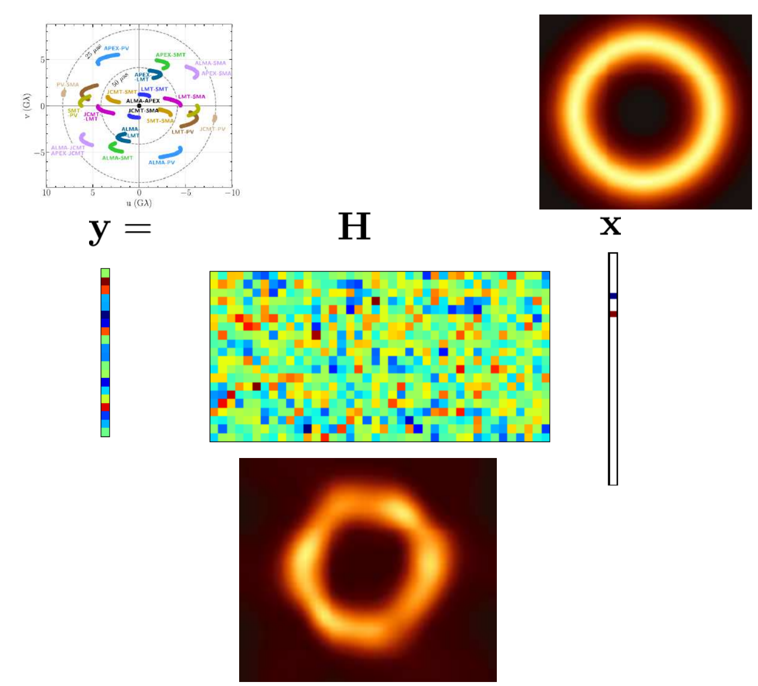
The unique features of physics applications and the power of physics principles offer compelling research opportunities to advance the field of AI research itself

Sparse Coding Networks and Neuronal Source Separation (Ba)



$\Leftrightarrow$

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

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

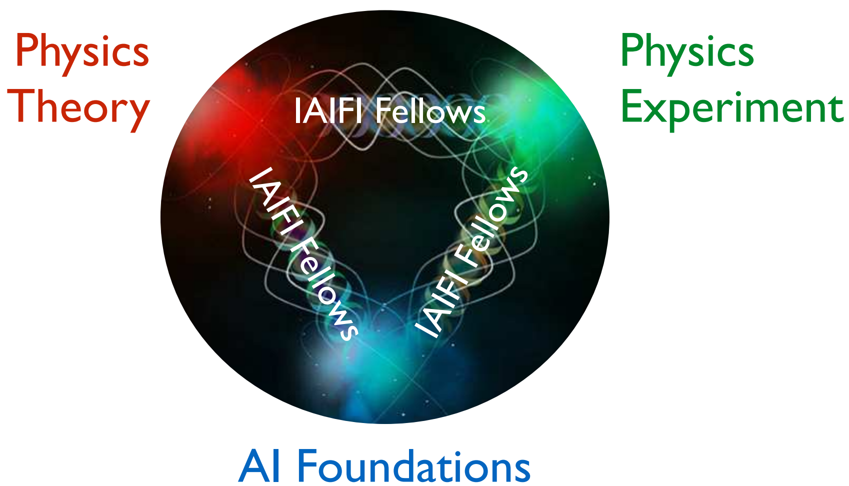
Programs like IAIFI Fellowships and Interdisciplinary PhD in Physics, Statistics & Data Science offer unique opportunities for early-career researchers to pursue their interests

IAIFI research has natural synergies with emerging interdisciplinary computation/data science institutes

"Machine Learning for the Physical Sciences" is growing dramatically, and now is the time to start thinking about new faculty hires in this area

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

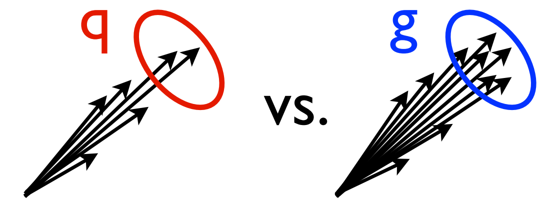
http://iaifi.org/

We look forward to collaborations and synergies with broader AI community

Backup Slides

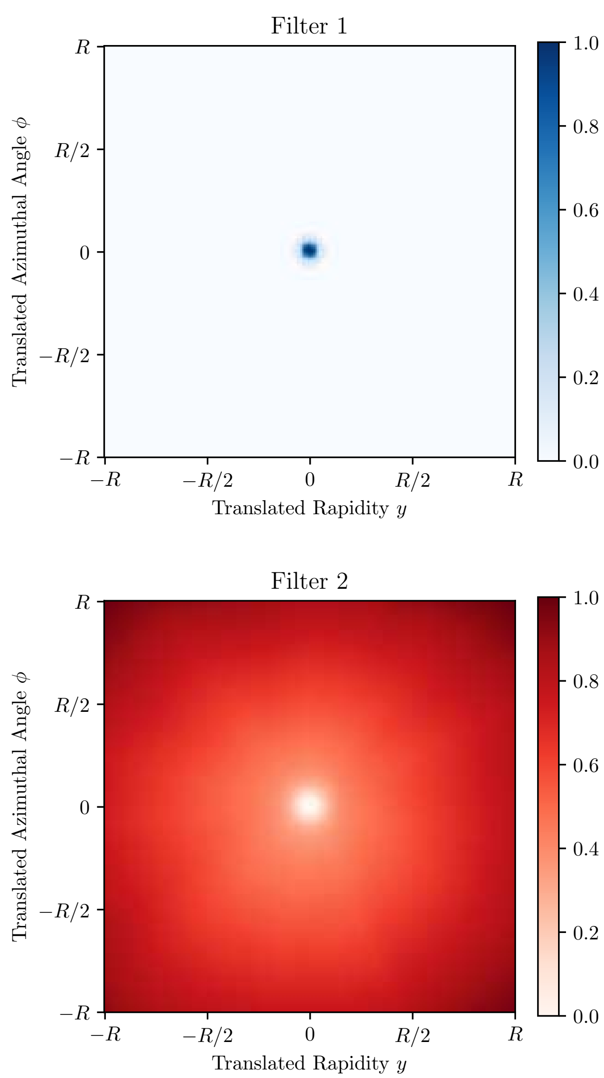
“Ok, but did you really learn something you didn’t already know?”

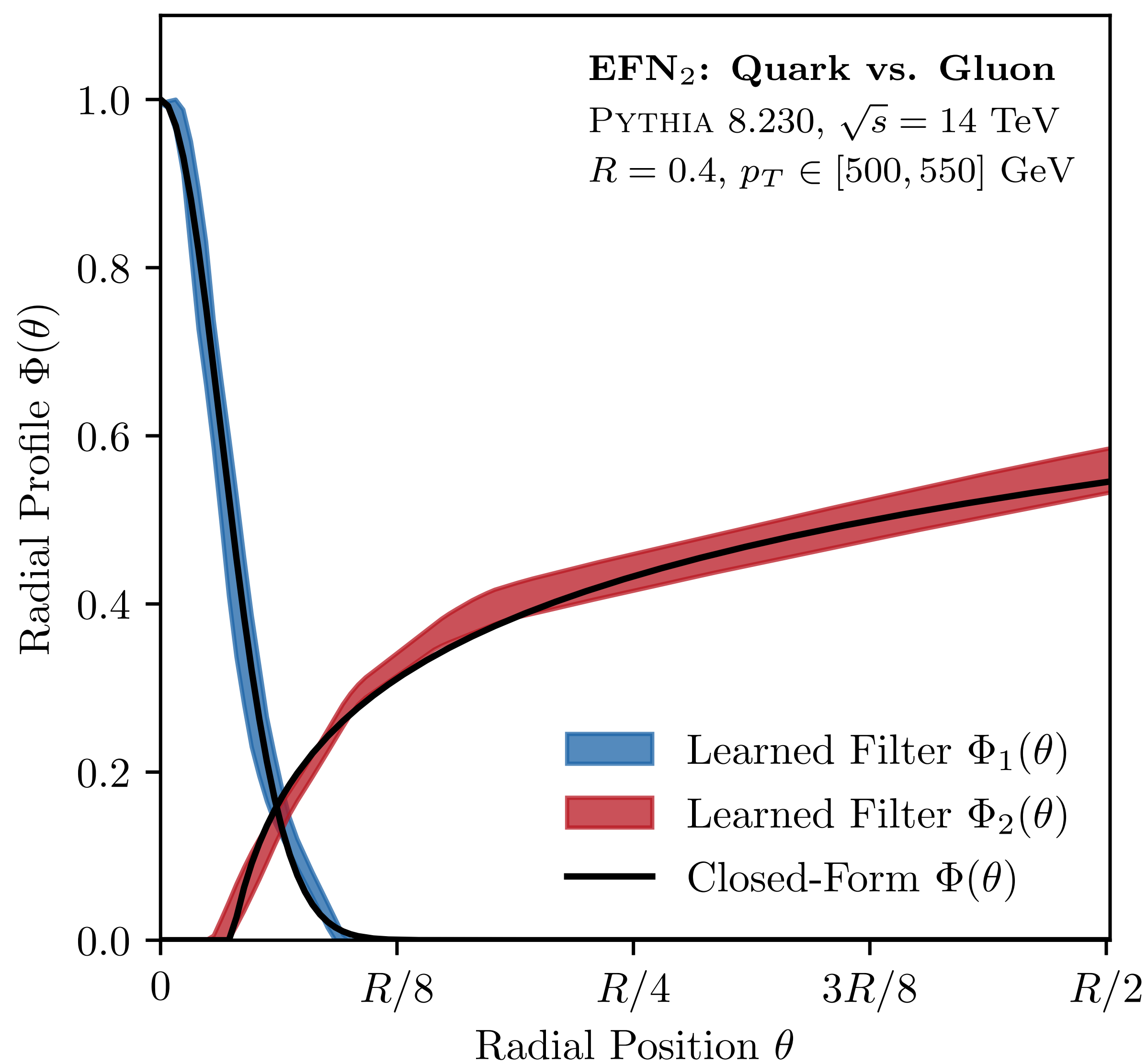
Learning from the Machine



For ℓ = 2 EFN, radial moments: $$\sum_{i \in \text{jet}} z_i \, f(\theta_i)$$

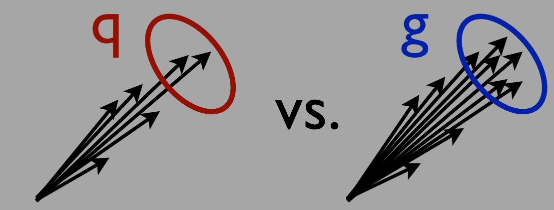
cf. Angularities: $f(\theta) = \theta^\beta$





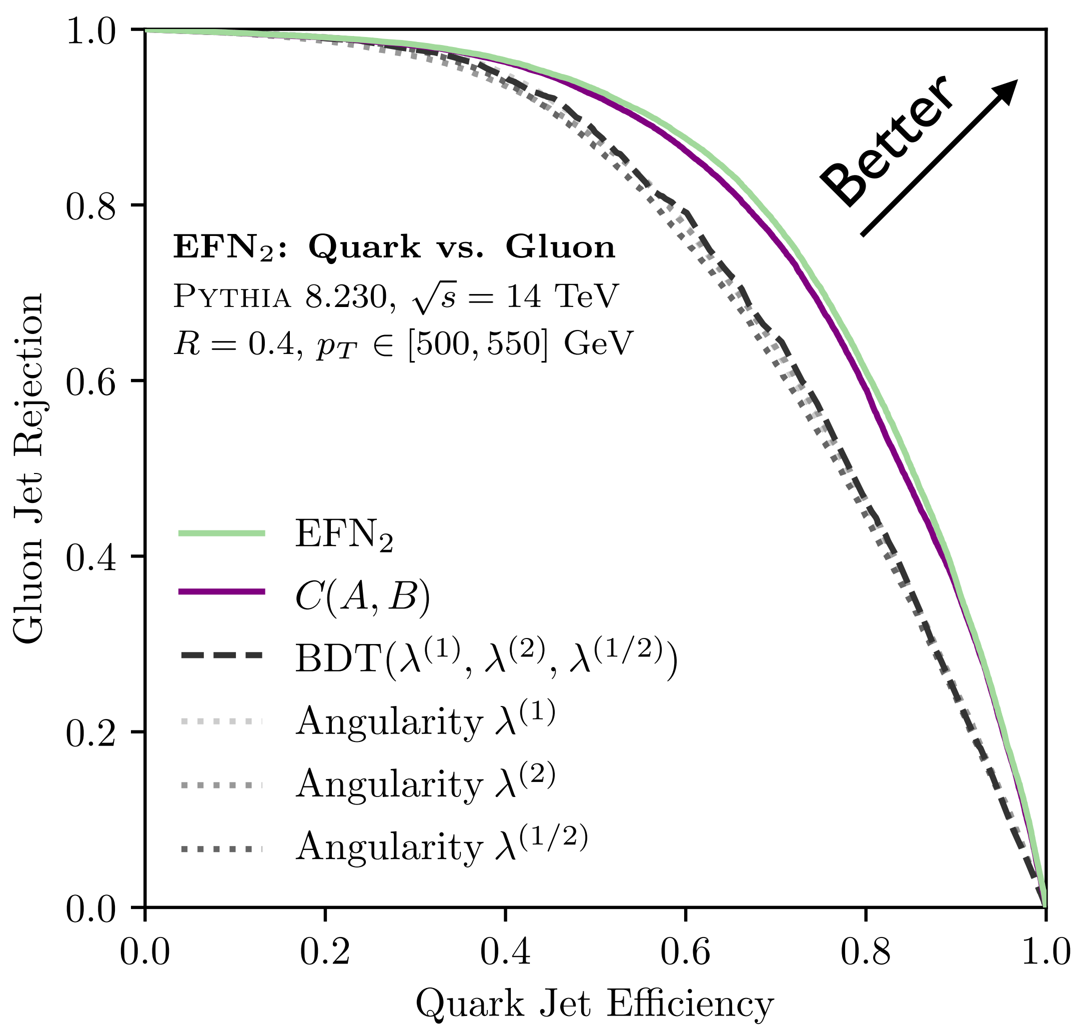
[Komiske, Metodiev, JDT, JHEP 2019;
cf. Larkoski, JDT, Waalewijn, JHEP 2014; using Berger, Kucs, Sterman, PRD 2003; Ellis, Vermilion, Walsh, Hornig, Lee, JHEP 2010]

Learning from the Machine



For ℓ = 2 EFN, radial moments: $\sum_{i \in \text{jet}} z_i f(\theta_i)$

cf. Angularities:
$f(\theta) = \theta^\beta$



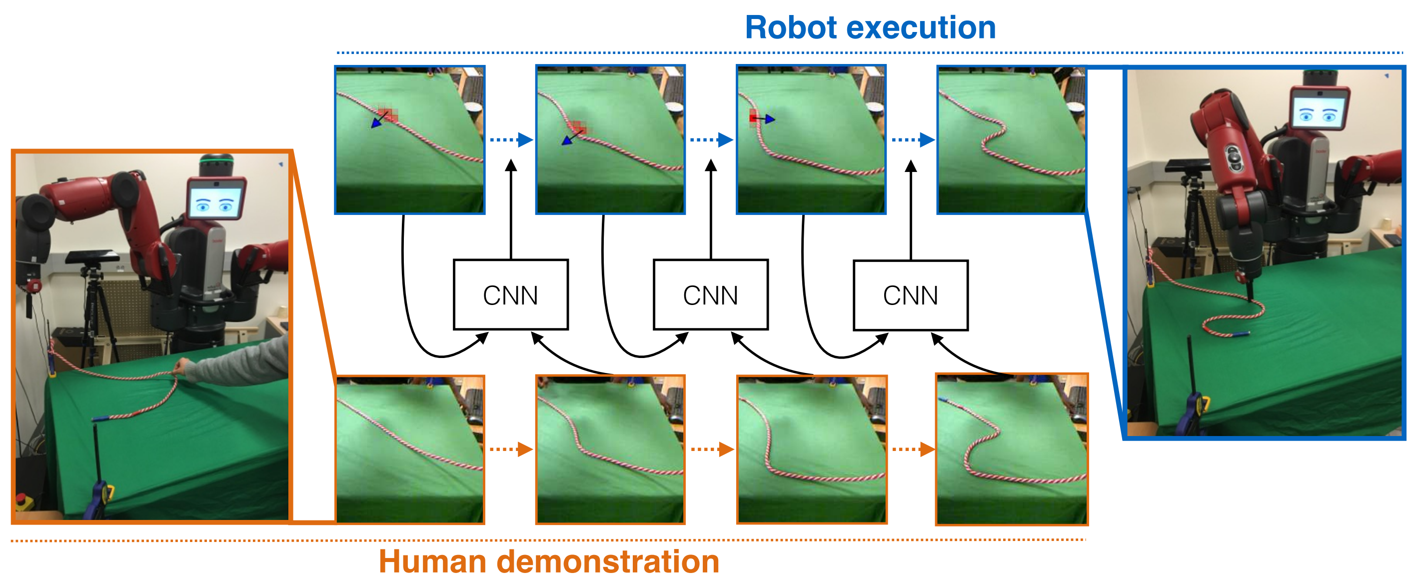
EFN outperformed a domain expert (i.e. me)

But we could reverse engineer the machine

[Komiske, Metodiev, JDT, JHEP 2019;
cf. Larkoski, JDT, Waalewijn, JHEP 2014; using Berger, Kucs, Sterman, PRD 2003; Ellis, Vermilion, Walsh, Hornig, Lee, JHEP 2010]

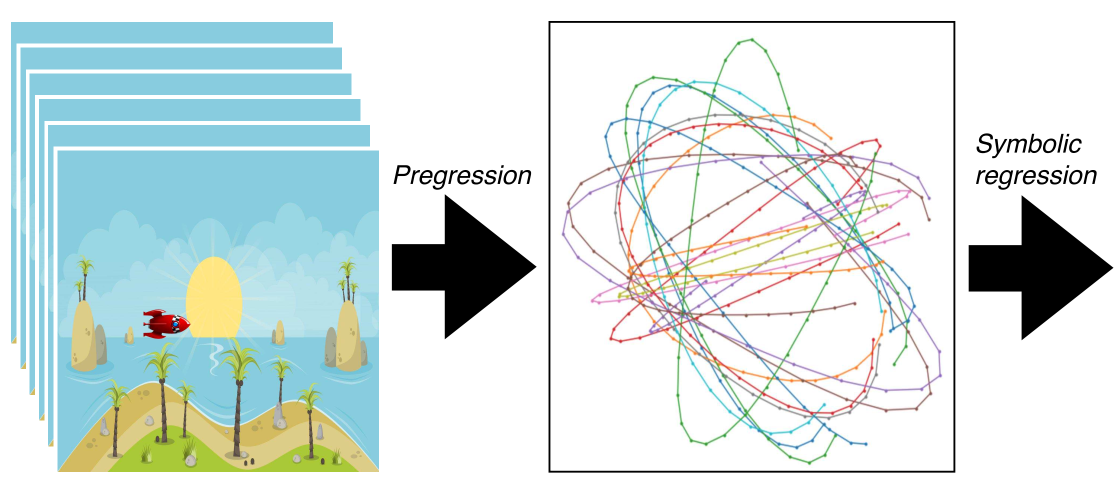
Learning Physical Laws from Spatiotemporal Data

"Course 6" Strategy:



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

"Course 8" Strategy:



$$\begin{aligned}\ddot{x} &= -(x^2+y^2)x\\ \ddot{y} &= -(x^2+y^2)y\end{aligned}$$

[Udrescu, Tegmark, arXiv 2020]

IAIFI Activities & Synergies

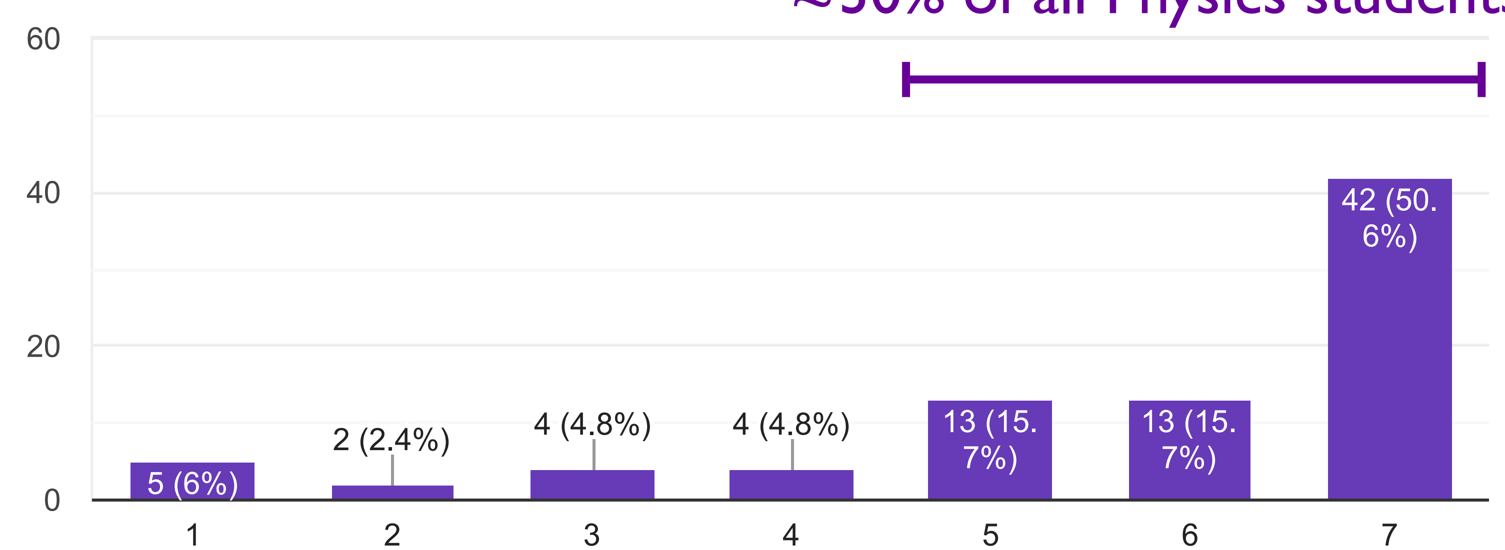
Interdisciplinary PhD in Physics, Statistics & Data Science

MIT Physics | MIT STATISTICS + DATA SCIENCE CENTER

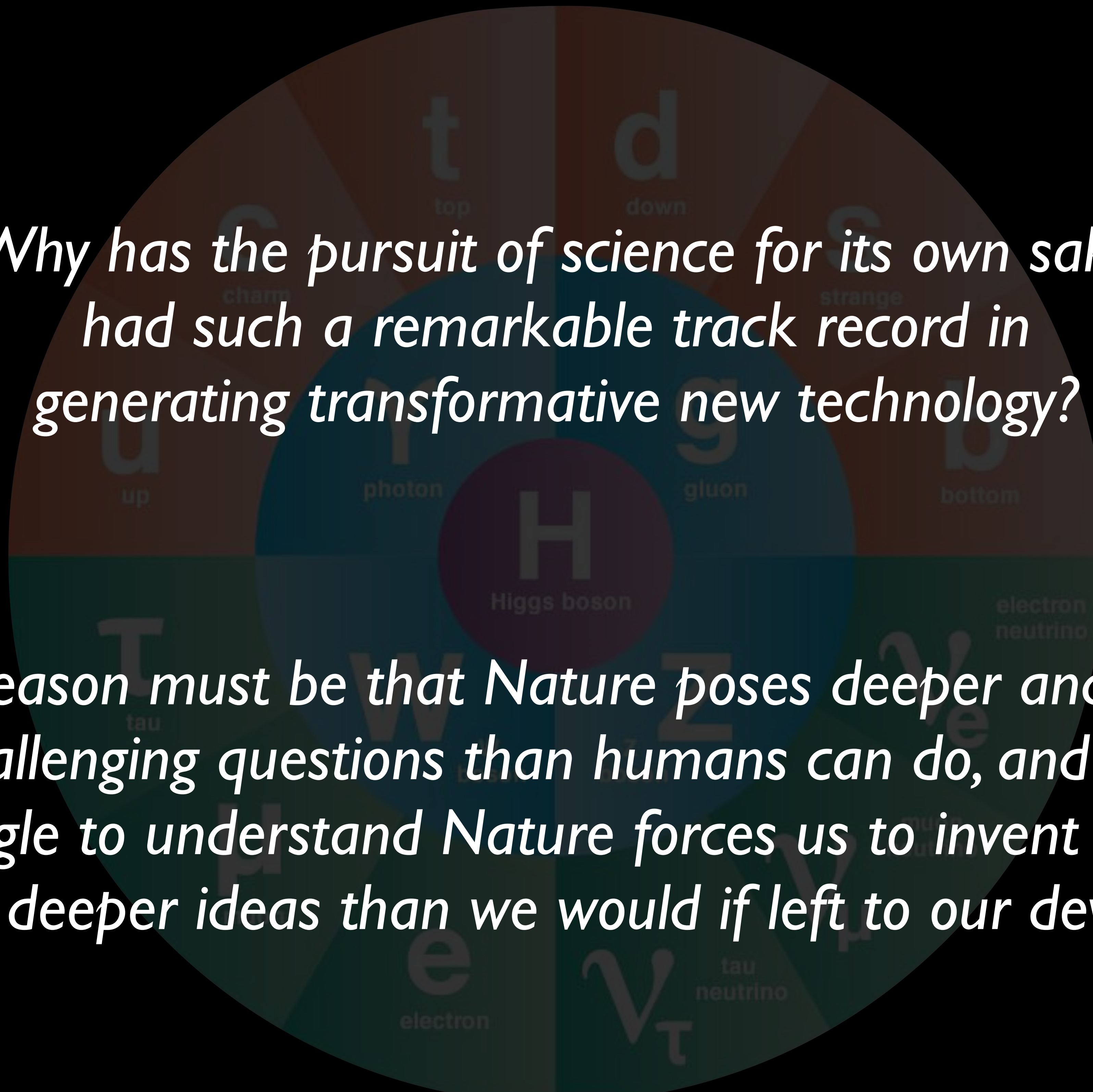
This interdisciplinary degree would have a number of requirements, in addition to the standard requirements for the MIT Physics PhD. How interested would you be in submitting and defending a PhD thesis that uses statistical methods in a substantial way?

83 responses

≈30% of all Physics students (!)



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



Why has the pursuit of science for its own sake had such a remarkable track record in generating transformative new technology?

The reason must be that Nature poses deeper and more challenging questions than humans can do, and the struggle to understand Nature forces us to invent better and deeper ideas than we would if left to our devices.

[David Gross (2004 Nobel Laureate in Physics), IJMPA 2016]