Collision Course

Particle Physics meets Machine Learning

Jesse Thaler

MIT

8.S50 — January 26, 2022

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

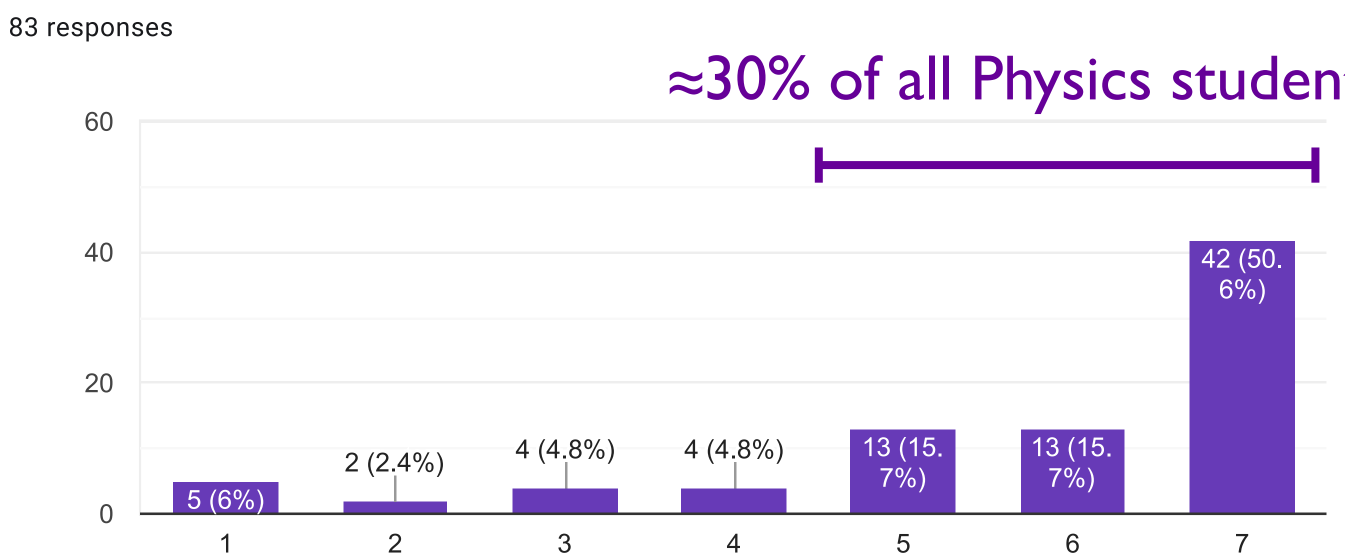
Advance physics knowledge — from the smallest building blocks of nature to the largest structures in the universe — and galvanize AI research innovation

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

New! PhD in Physics, Statistics & Data Science

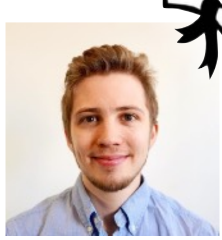
≈ Physics PhD + 4 courses (probability, statistics, computation, data analysis)

How interested would you be in submitting and defending a PhD thesis that uses statistical methods in a substantial way?



≈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."

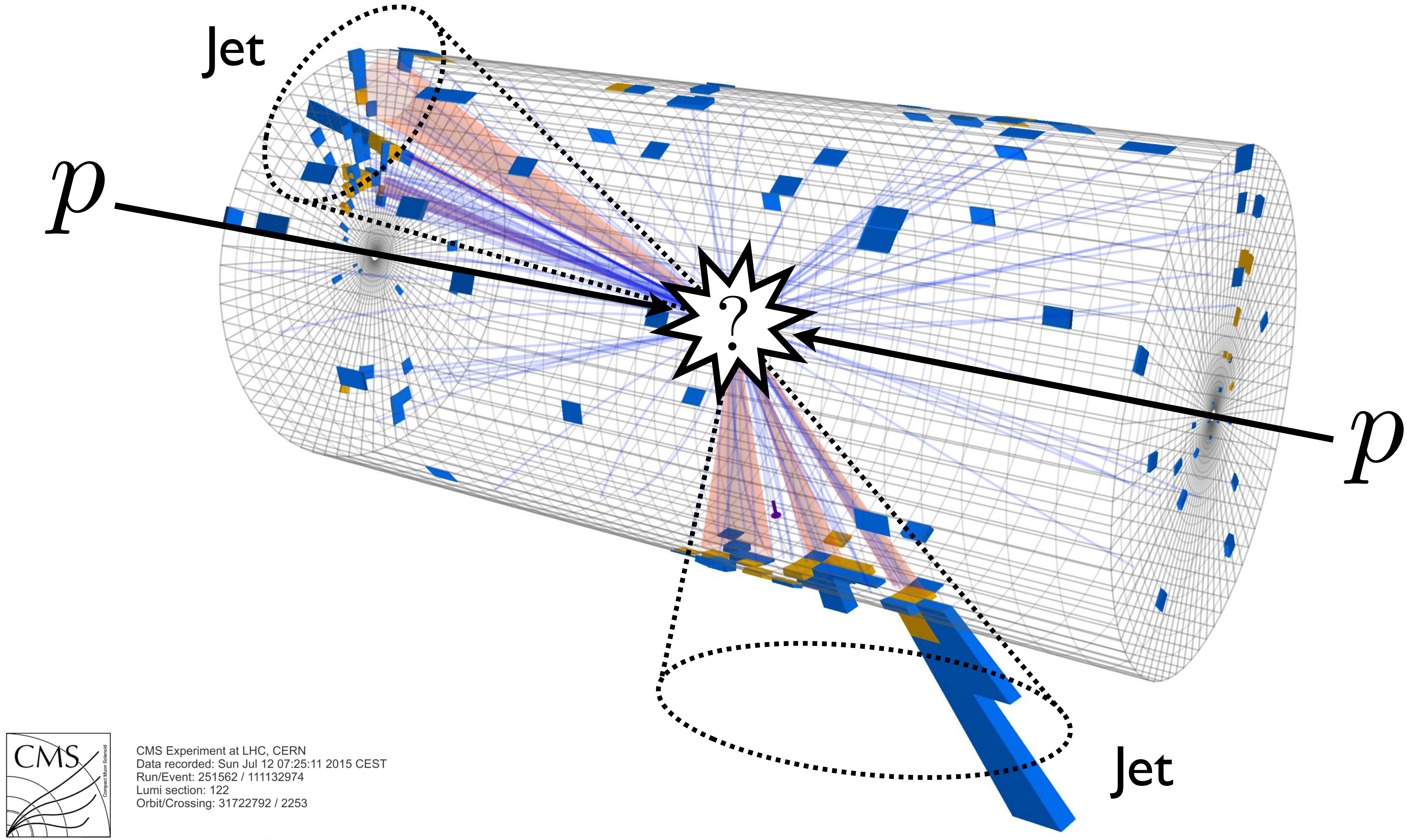


Congratulations,
Dr. Constantin Weisser!
(March 30, 2021)

[https://physics.mit.edu/academic-programs/graduate-students/psds-phd/]

“Collision Course”

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



“Collision Course”

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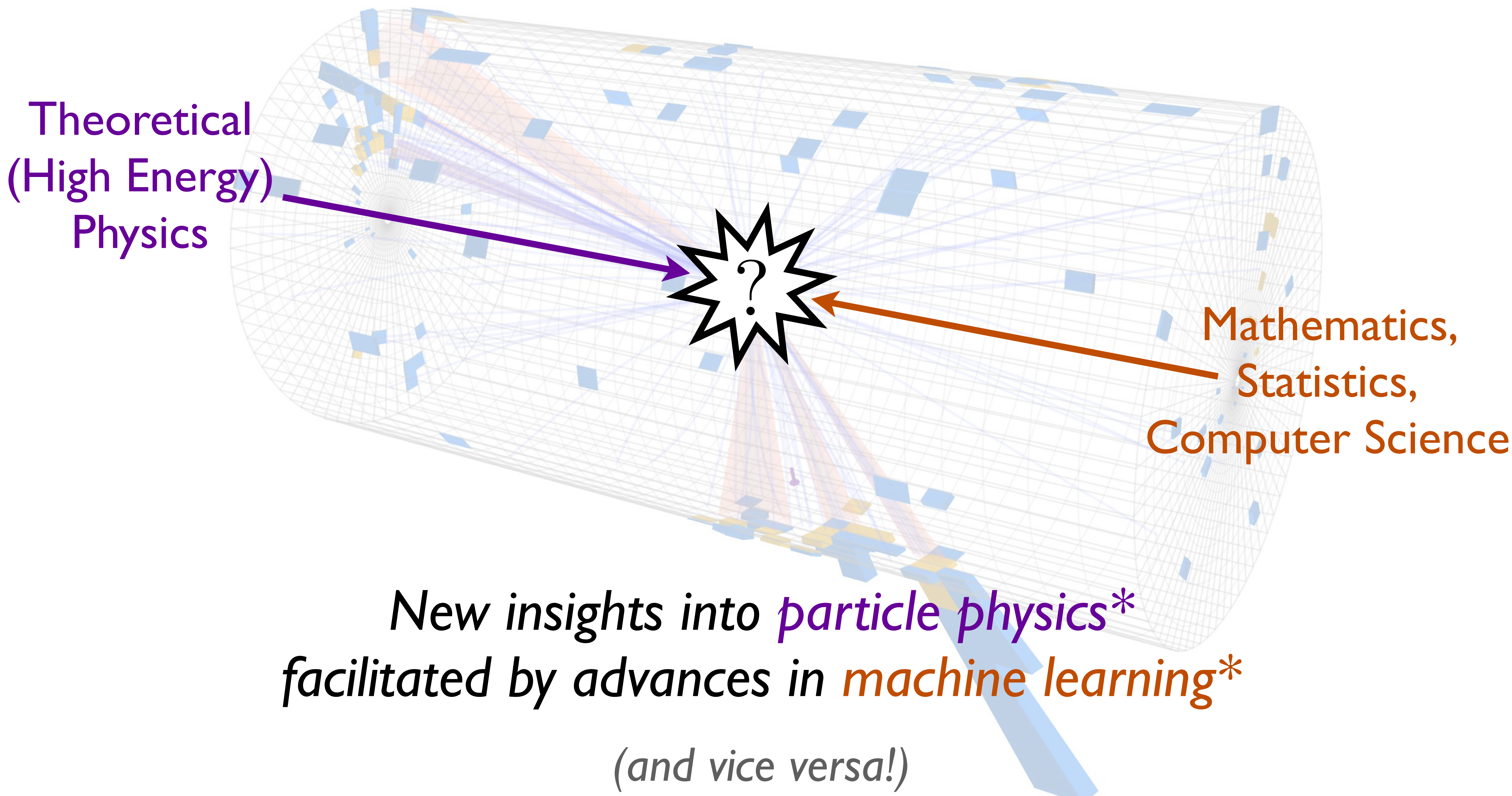
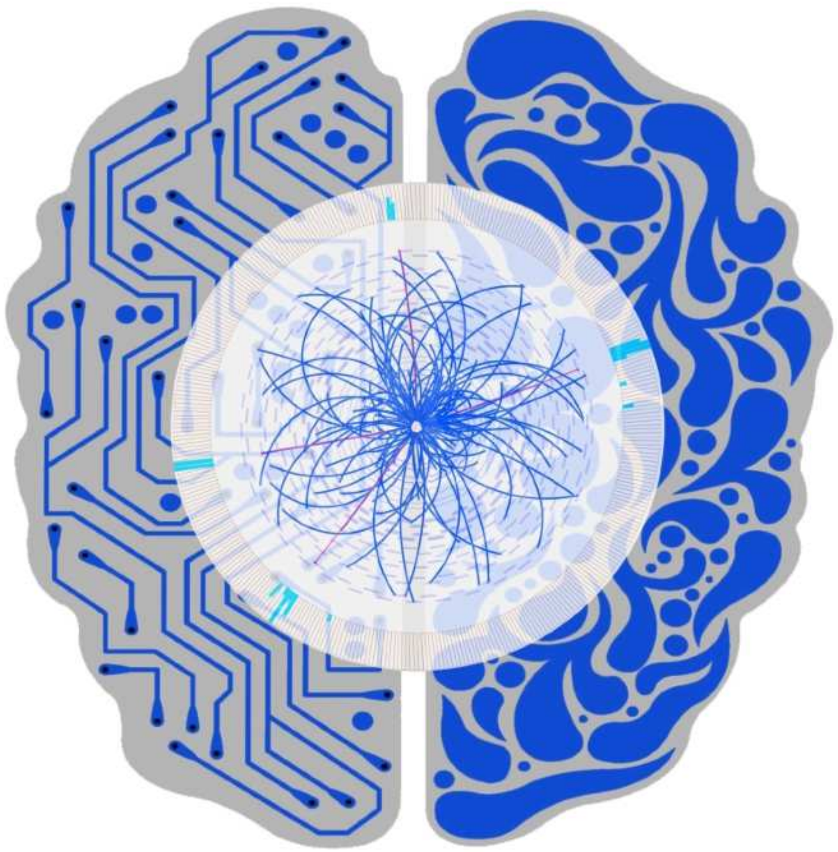


*New insights into particle physics**
*facilitated by advances in machine learning**

(and vice versa!)



Can we teach a machine to “think” like a physicist?

The New York Times

By Dennis Overbye

Nov. 23, 2020

Can a Computer Devise a Theory of Everything?

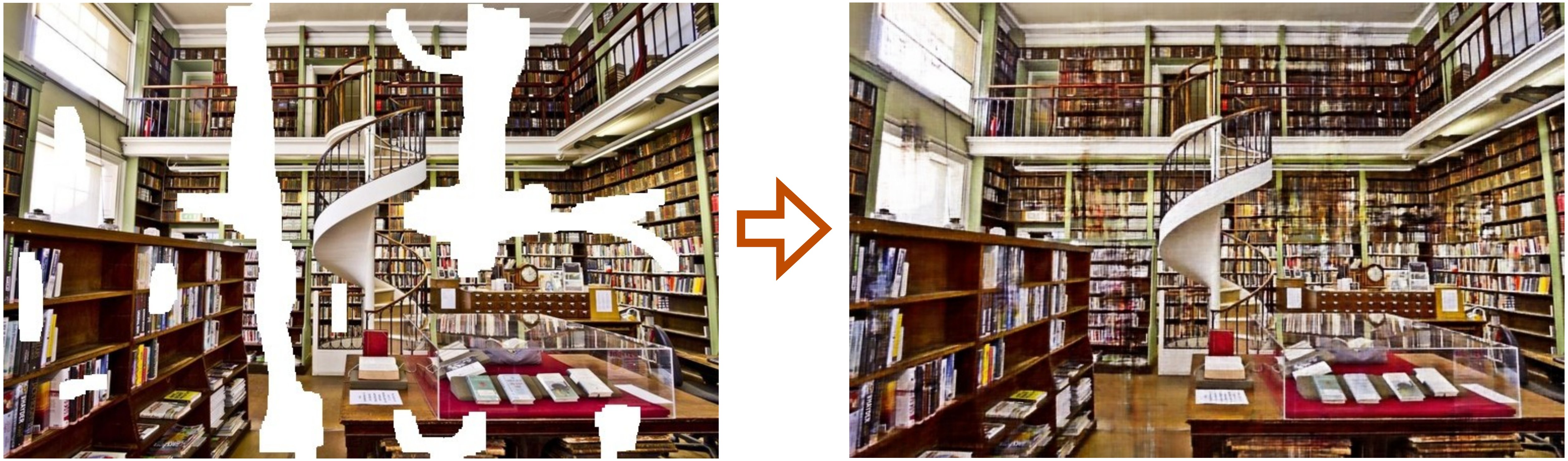
AI^2: Ab Initio Artificial Intelligence

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, …

Deep Learning

E.g. Inpainting

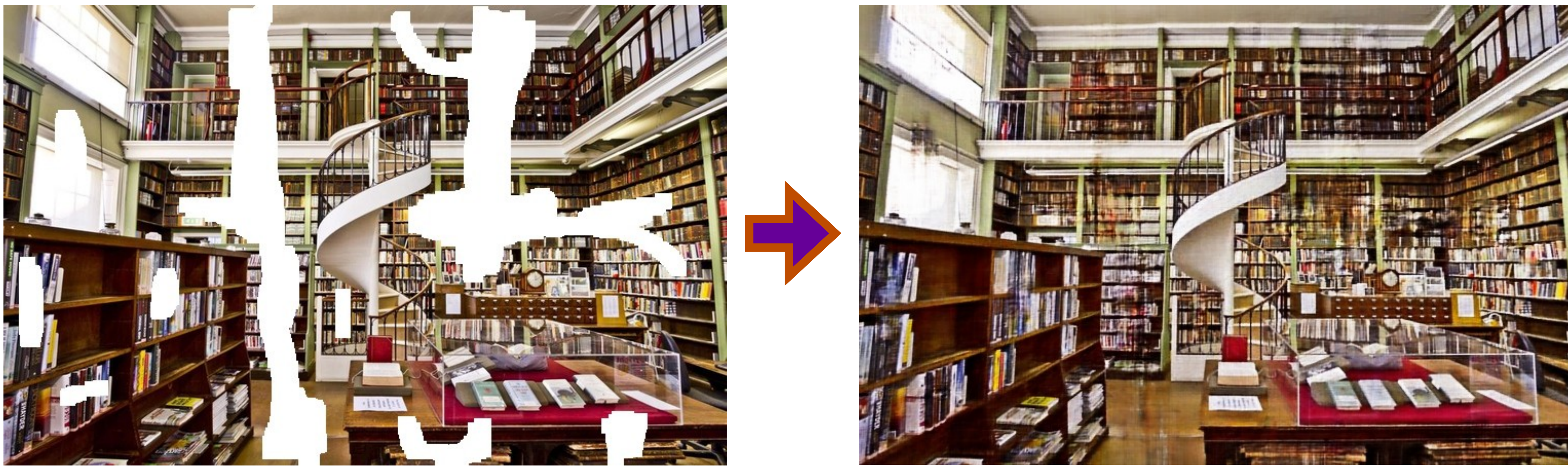


increased computational power and large data sets

[Ulyanov, Vedaldi, Lempitsky, CVPR 2018]

Deep Learning meets Deep Thinking

E.g. Inpainting



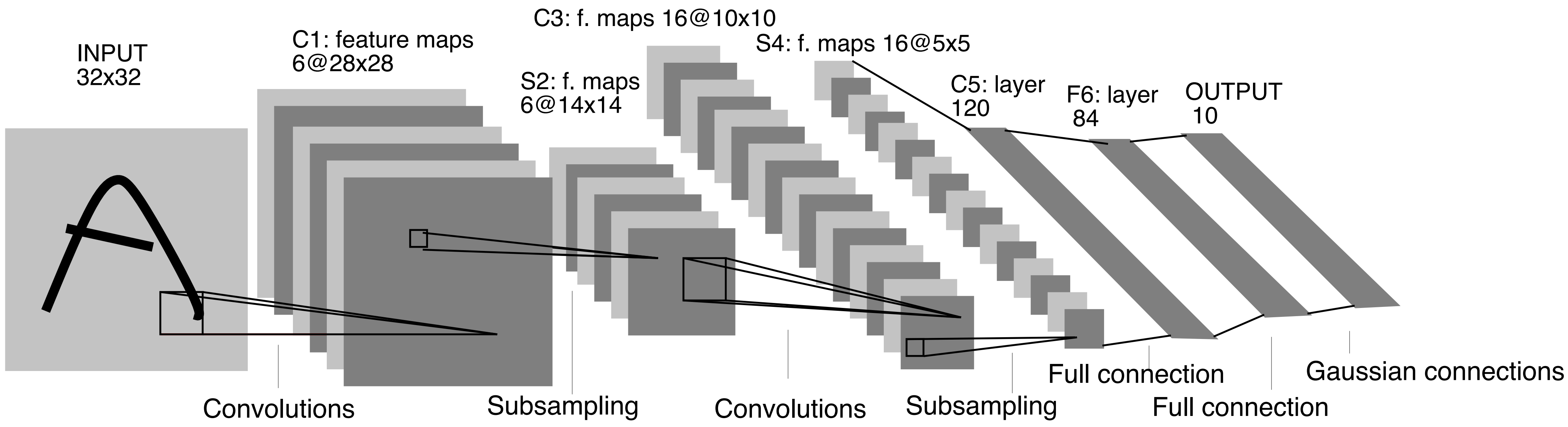
Using randomly initialized neural network (!)

Progress made by understanding the structure of problems

(not just increased computational power and large data sets)

[Ulyanov, Vedaldi, Lempitsky, CVPR 2018]

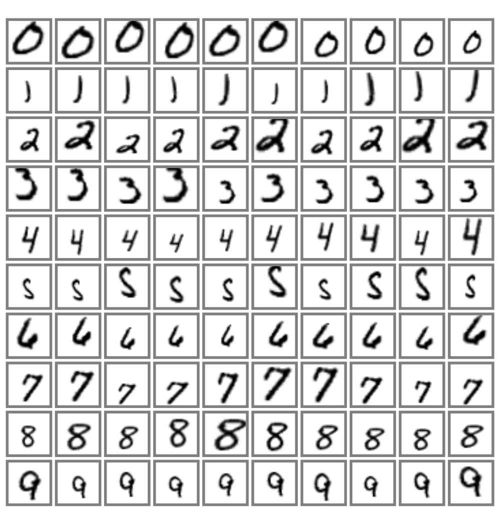
Symmetries of Convolutional NNs



Explores different length scales

Enforces Translation Equivariance

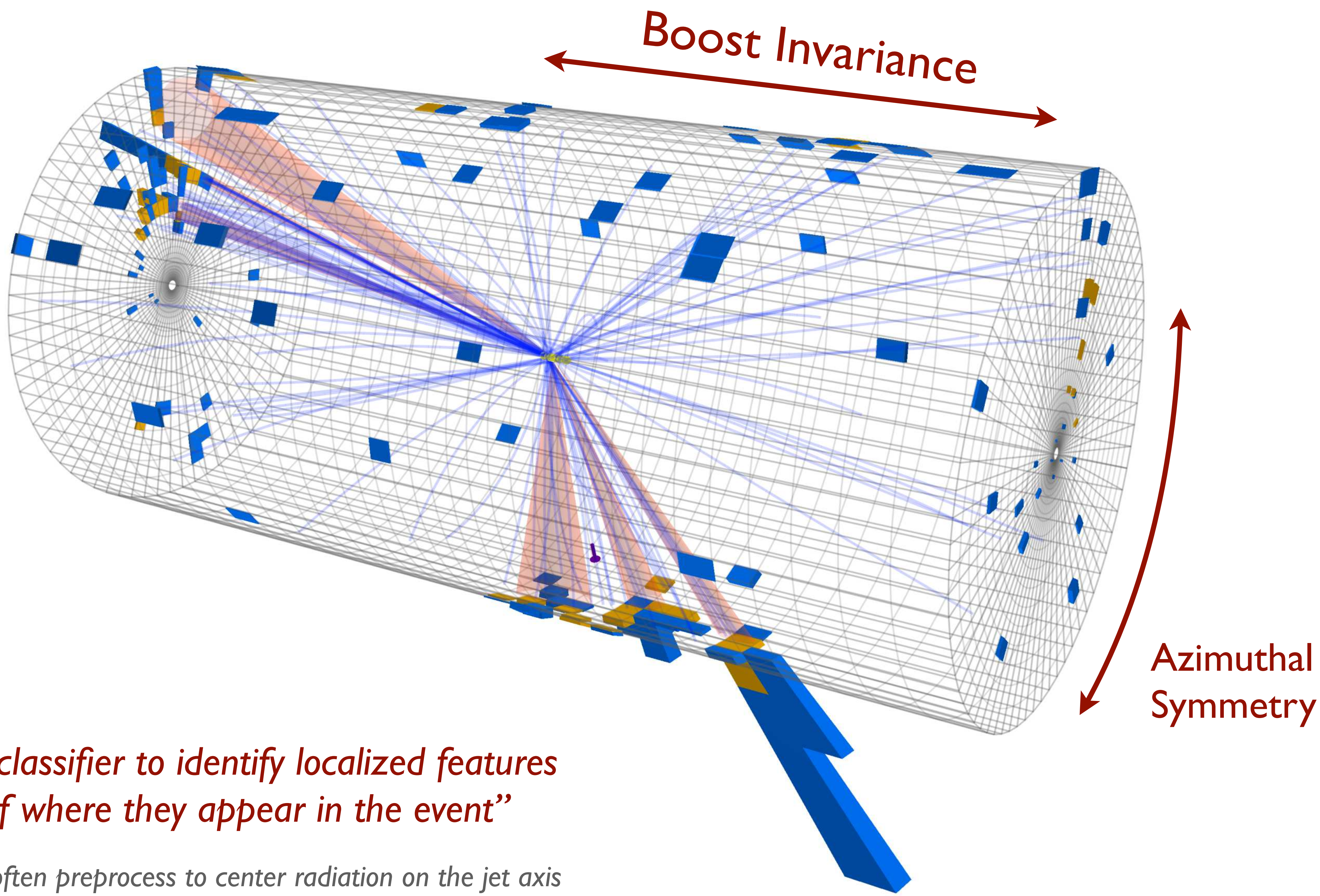
= Covariance for a Physicist



"I want my classifier to identify localized features regardless of where they appear in the image"

[image from LeCun, Bottou, Bengio, Haffner, 1998]

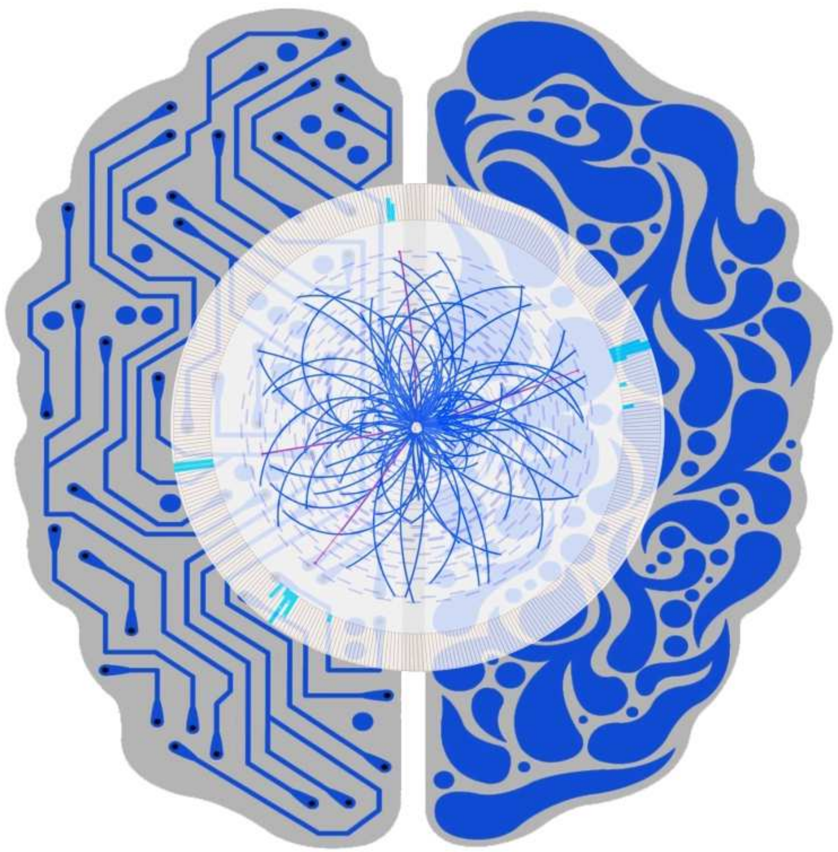
Symmetries of Collision Events



"I want my classifier to identify localized features regardless of where they appear in the event"

In practice, we often preprocess to center radiation on the jet axis

[image from CMS, 2015]



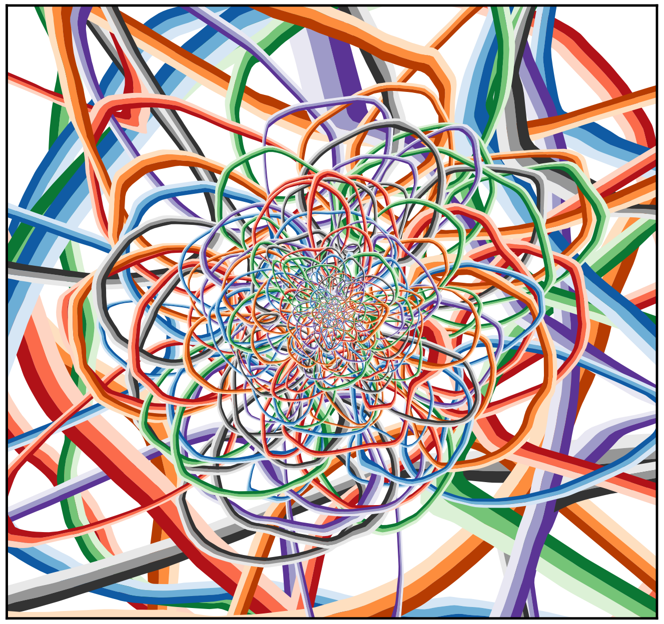
Can we encode known structures of particle physics data into a neural network architecture?

AI^2: 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

= AI^2 — Cross-cutting research across disciplines

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Likelihood Ratio Trick

Many particle physics problems can be expressed in this form!

Key example of simulation-based inference

Goal: Estimate p(x) / q(x)

Training Data: Finite samples P and Q

Learnable Function: f(x) parametrized by, e.g., neural networks

Loss Function(al): $$L = -\big\langle \log f(x) \big\rangle_P + \big\langle f(x) - 1 \big\rangle_Q$$

Asymptotically: $$\arg\min_{f(x)} L = \frac{p(x)}{q(x)}$$ *Likelihood ratio*

$$-\min_{f(x)} L = \int \mathrm{d}x\, p(x) \log \frac{p(x)}{q(x)}$$ *Kullback–Leibler divergence*

[see e.g. D'Agnolo, Wulzer, PRD 2019; simulation-based inference in Cranmer, Brehmer, Louppe, PNAS 2020; relation to f-divergences in Nguyen, Wainwright, Jordan, AoS 2009]

Likelihood Ratio Trick

Key example of simulation-based inference

Many particle physics problems can be expressed in this form!

Asymptotically, same structure as Lagrangian mechanics!

Action: $$L = \int \mathrm{d}x\, \mathcal{L}(x)$$

Lagrangian: $$\mathcal{L}(x) = -p(x) \log f(x) + q(x)\big(f(x) - 1\big)$$

Euler-Lagrange: $$\frac{\partial \mathcal{L}}{\partial f} = 0$$

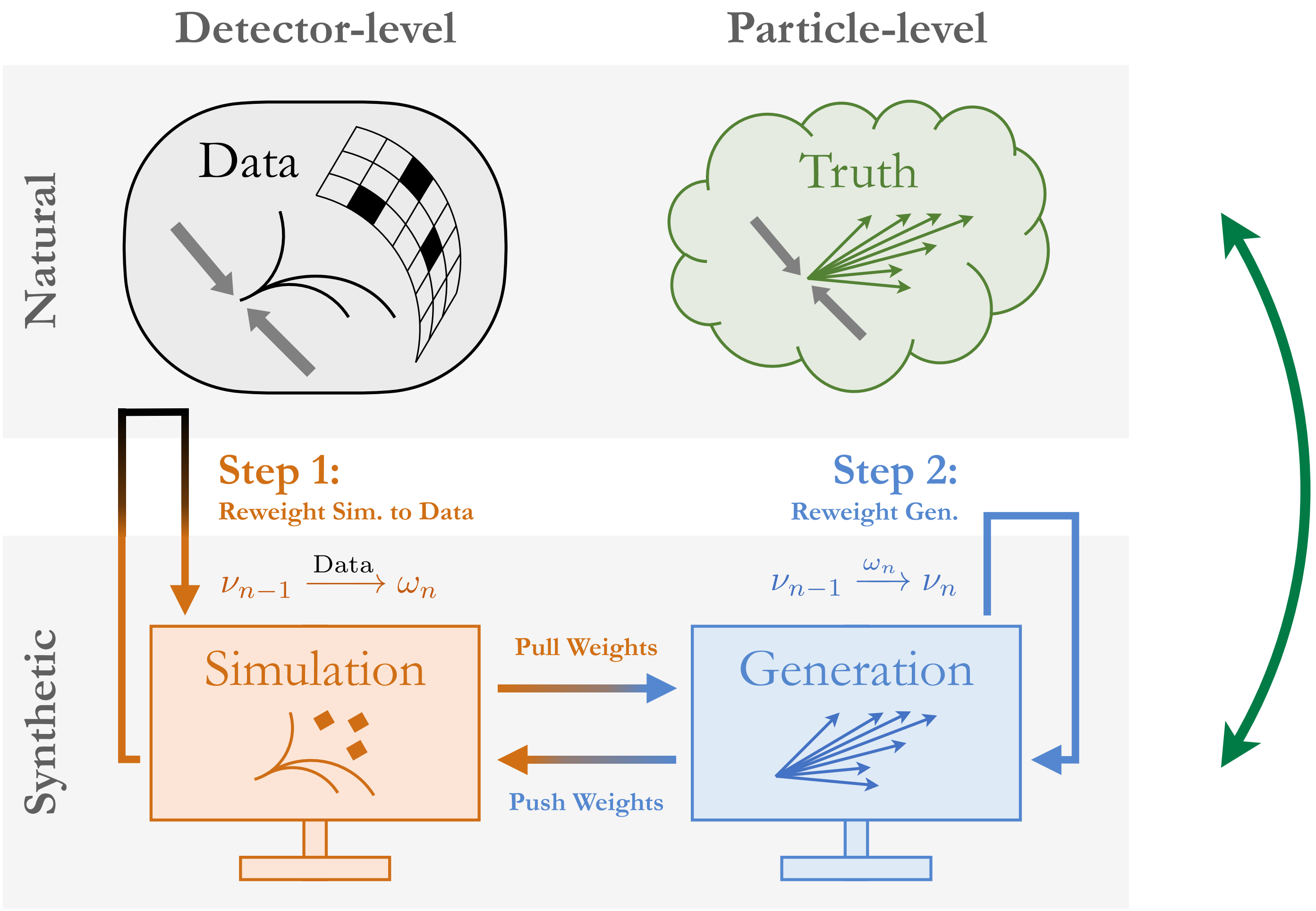
Solution: $$f(x) = \frac{p(x)}{q(x)}$$

Requires shift in focus from solving problems to specifying problems

[see e.g. D'Agnolo, Wulzer, PRD 2019; simulation-based inference in Cranmer, Brehmer, Louppe, PNAS 2020; relation to f-divergences in Nguyen, Wainwright, Jordan, AoS 2009]

Deconvolution with OmniFold

Multi-dimensional unbinned detector corrections via iterated application of likelihood ratio trick

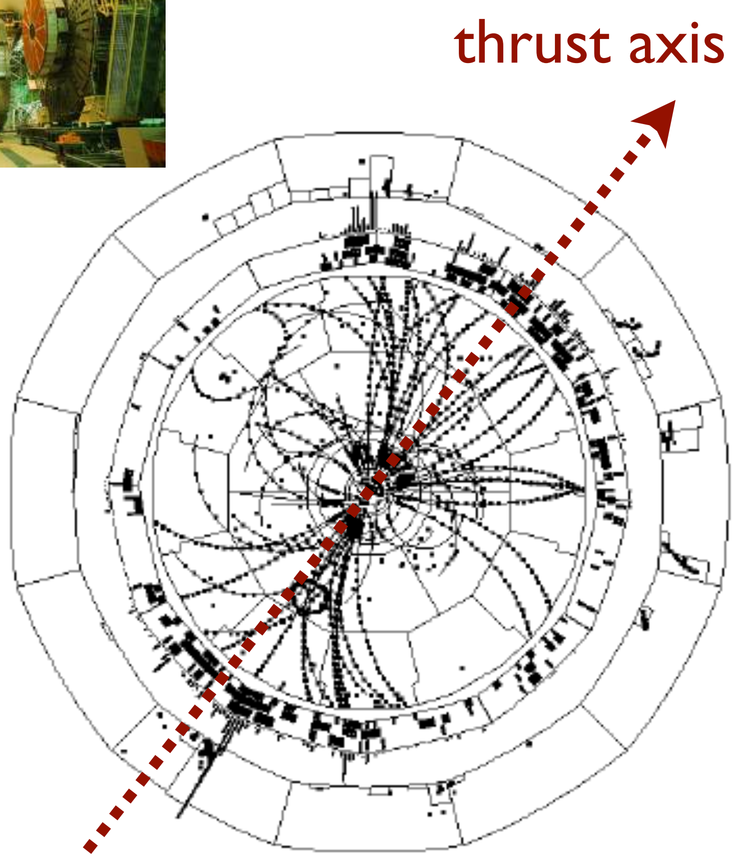


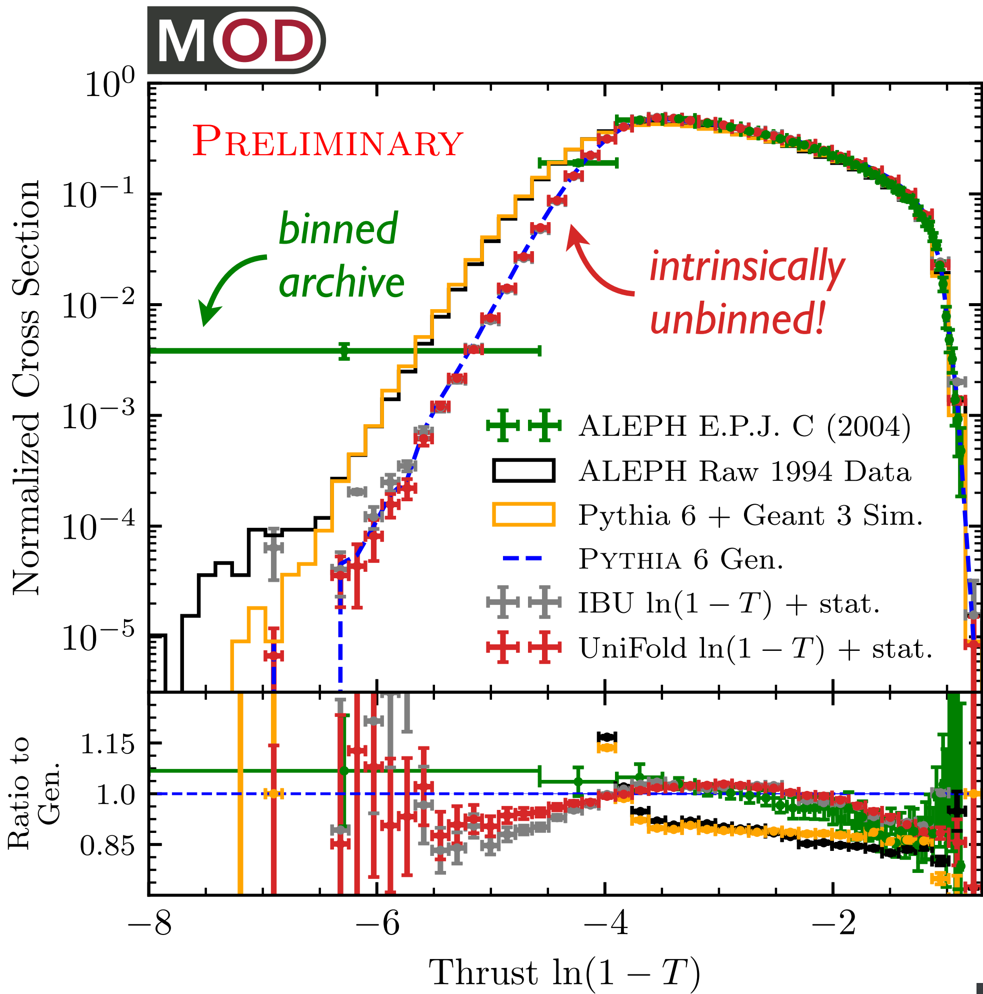
Use deep learning to compute reweighting factors

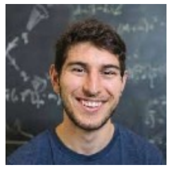
[Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020]
[see complimentary approach in Bellagente, et al., SciPost 2020]

Deconvolution with OmniFold

Back to the Future with ALEPH Archival Data







[talk by Badea, ICHEP 2020; cf. ALEPH, EPJC 2004]
[see also Badea, Baty, Chang, Innocenti, Maggi, McGinn, Peters, Sheng, JDT, Lee, PRL 2019]

[Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020]
[see complimentary approach in Bellagente, et al., SciPost 2020]

“What is the machine learning?”

For this loss function, an estimate of the likelihood ratio derived from sampled data and regularized by the network architecture and training paradigm

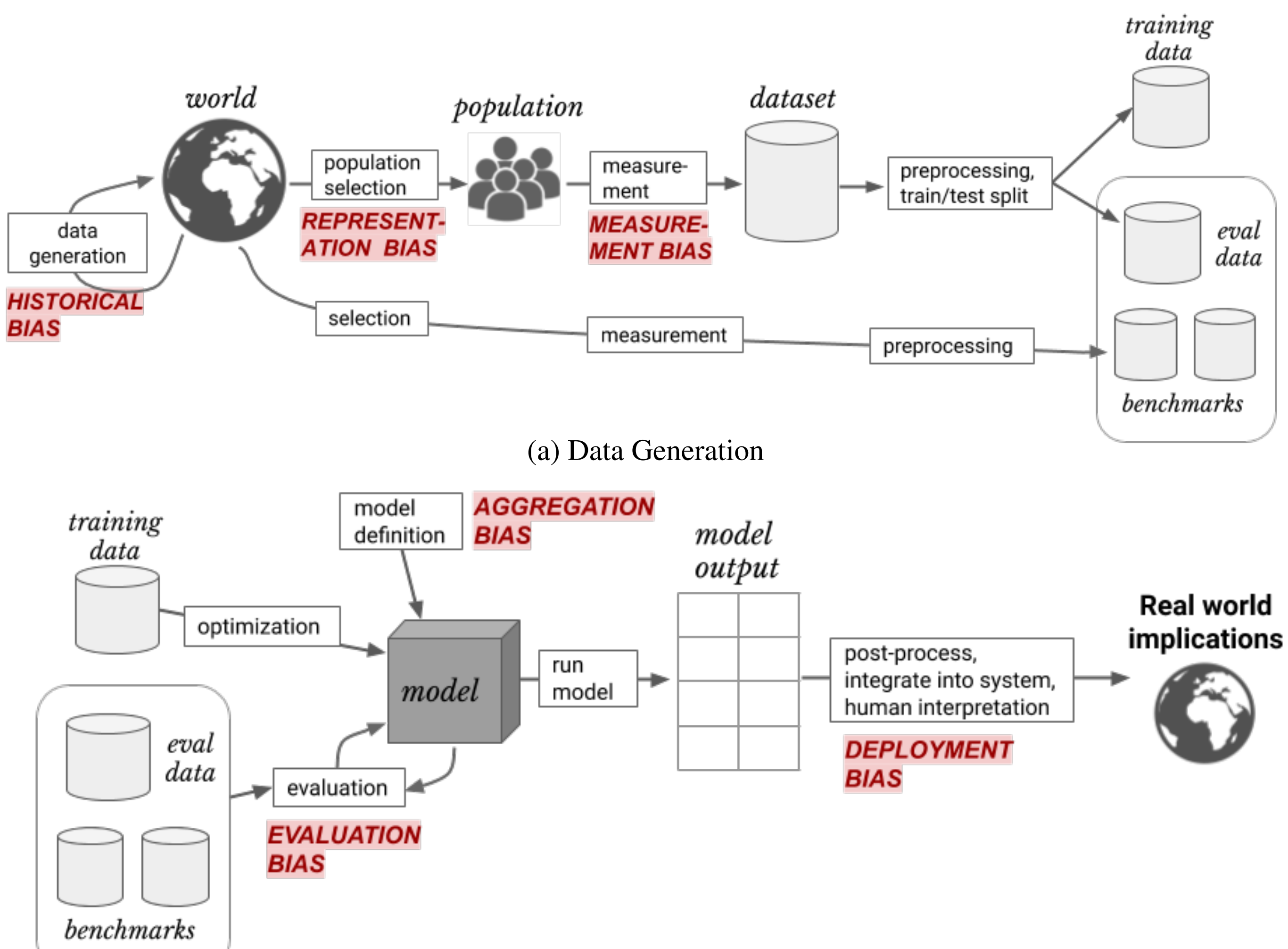
“But where’s the physics?!”

In the choice of loss function, data samples, network architecture, and training paradigm

“…”

Many Reasons to be Wary!

“A Framework for Understanding Unintended Consequences of Machine Learning”



(a) Data Generation

(b) Model Building and Implementation

1. **Historical bias** arises when there is a misalignment between world as it is and the values or objectives to be encoded and propagated in a model. It is a normative concern with the state of the world, and exists even given perfect sampling and feature selection.
2. **Representation bias** arises while defining and sampling a development population. It occurs when the development population under-represents, and subsequently fails to generalize well, for some part of the use population.
3. **Measurement Bias** arises when choosing and measuring features and labels to use; these are often proxies for the desired quantities. The chosen set of features and labels may leave out important factors or introduce group- or input-dependent noise that leads to differential performance.
4. **Aggregation bias** arises during model construction, when distinct populations are inappropriately combined. In many applications, the population of interest is heterogeneous and a single model is unlikely to suit all subgroups.
5. **Evaluation bias** occurs during model iteration and evaluation. It can arise when the testing or external benchmark populations do not equally represent the various parts of the use population. Evaluation bias can also arise from the use of performance metrics that are not appropriate for the way in which the model will be used.
6. **Deployment Bias** occurs after model deployment, when a system is used or interpreted in inappproprіate ways.

For collider physics, “bias” ≈ “systematic uncertainty”

[h/t David Kaiser, MIT SERC; Suresh, Guttag, arXiv 2019]

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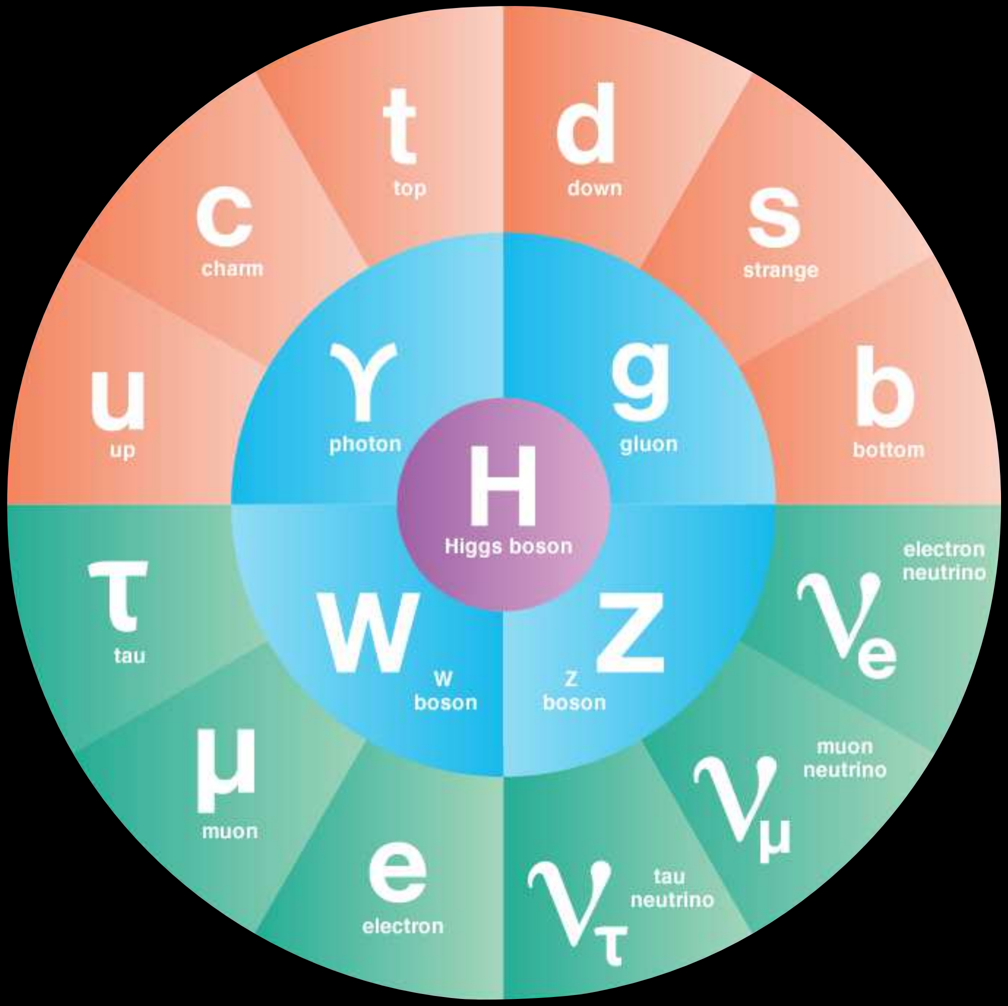
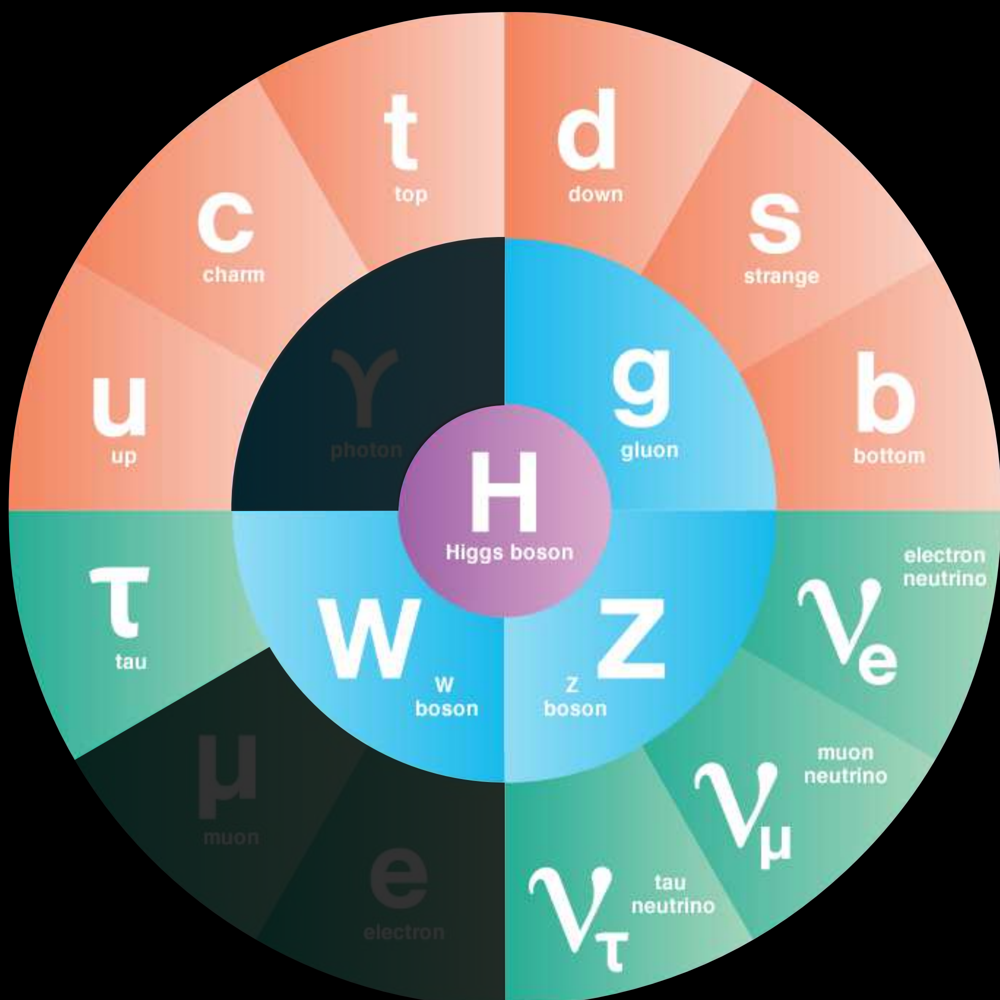
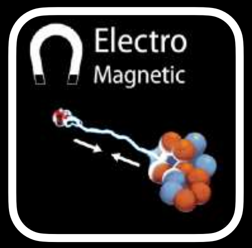
Particle Physics 101

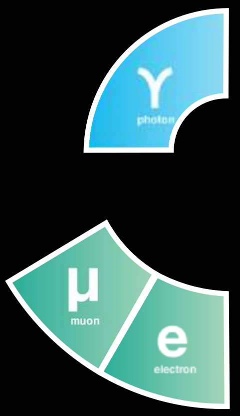


Particle Physics 101



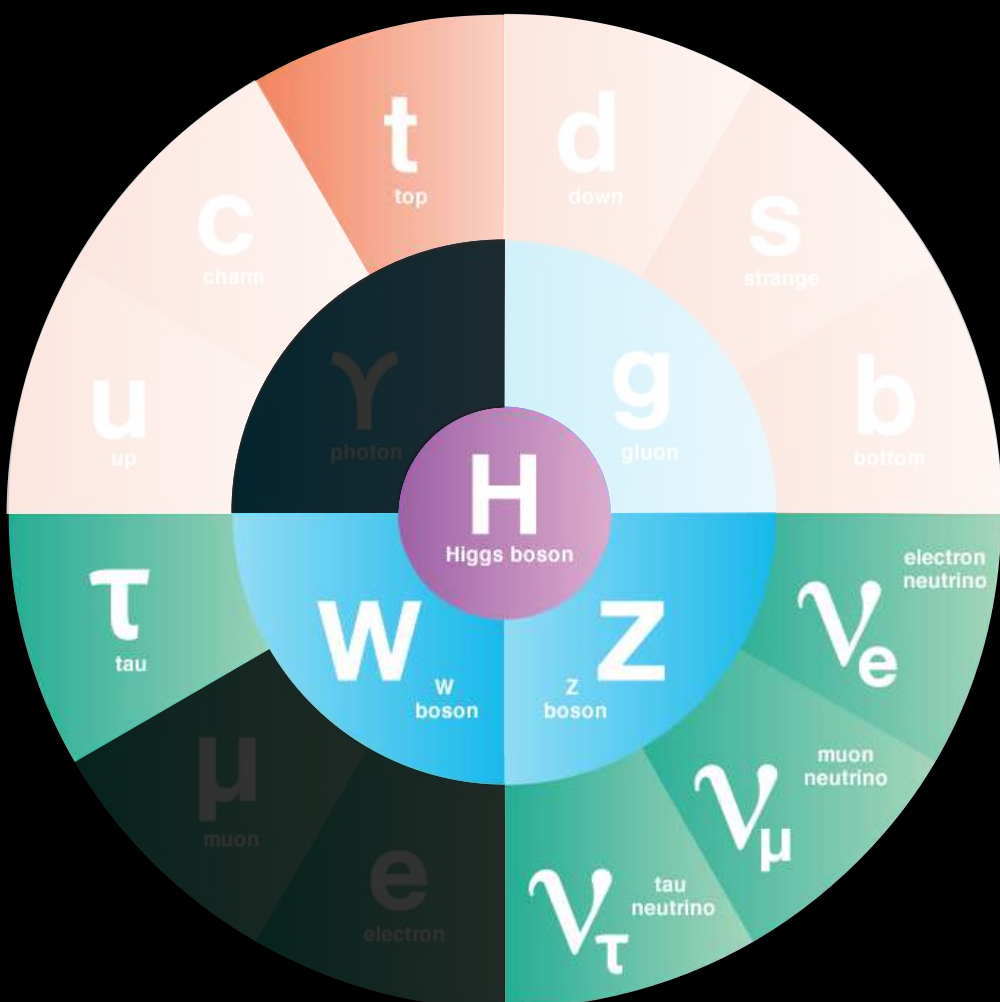
⇨

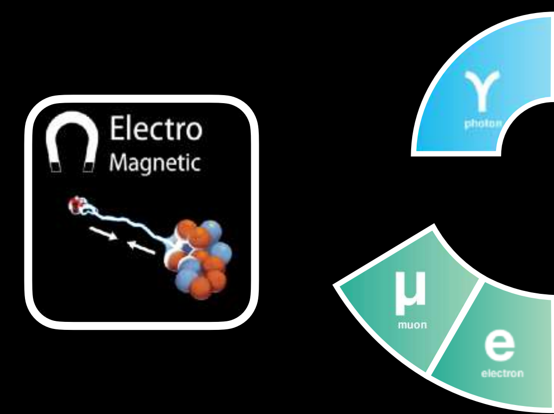




γ	photon	elementary
$e^\pm$	electron	
$\mu^\pm$	muon	

Particle Physics 101



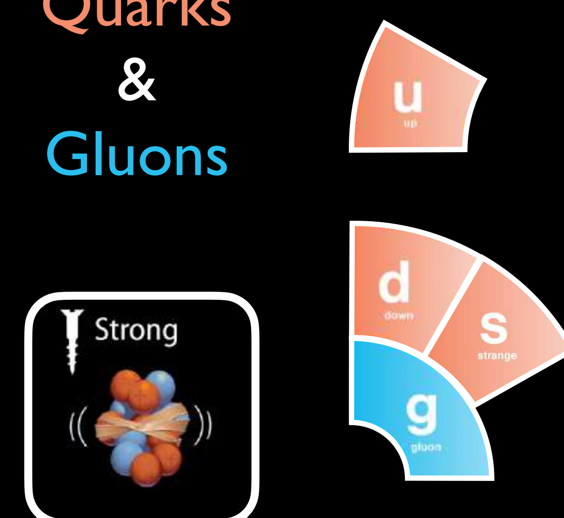


QCD Confinement

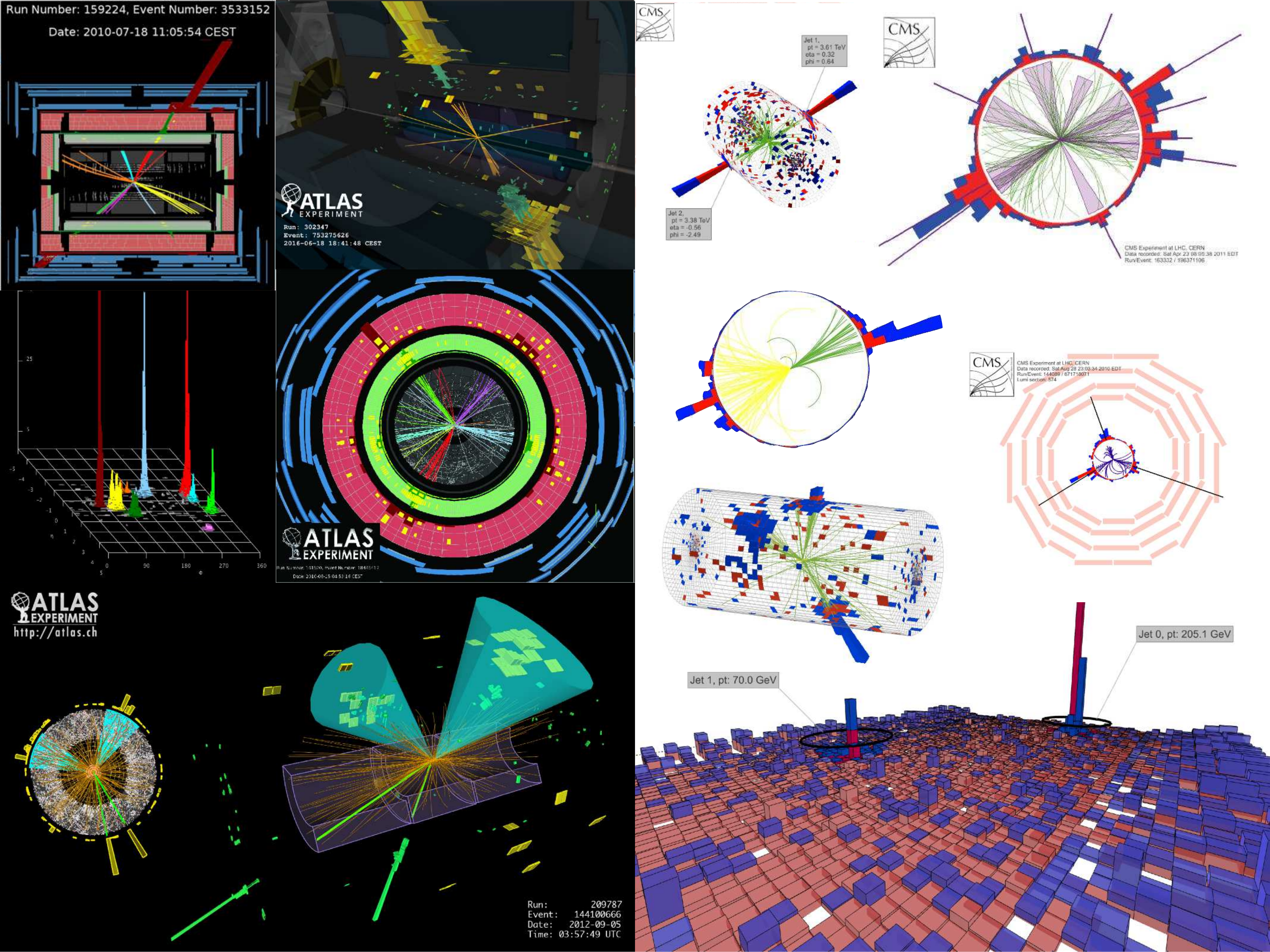
Quarks

&

Gluons



γ	photon	elementary
$e^{\pm}$	electron	
$\mu^{\pm}$	muon	
$\pi^{\pm}$	pion	composite
$K^{\pm}$	kaon	
K_L^0	K-long	
$p/\overline{p}$	proton	
$n/\overline{n}$	neutron	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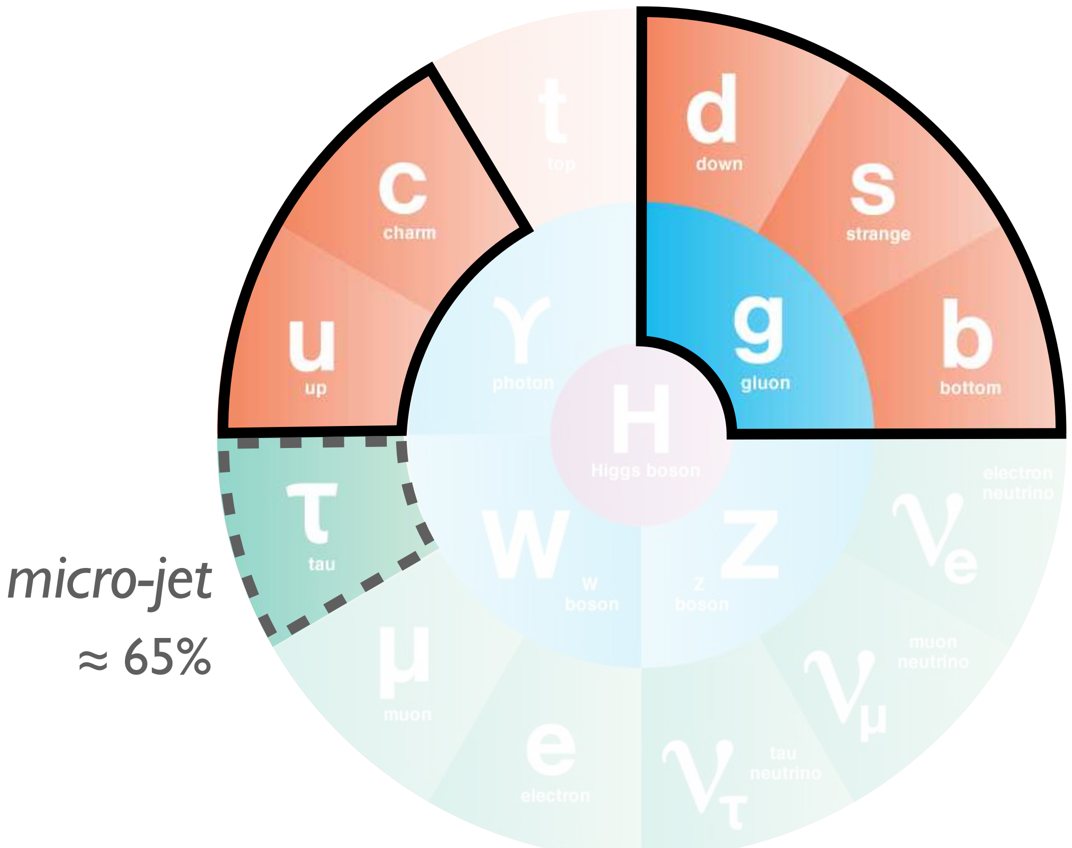
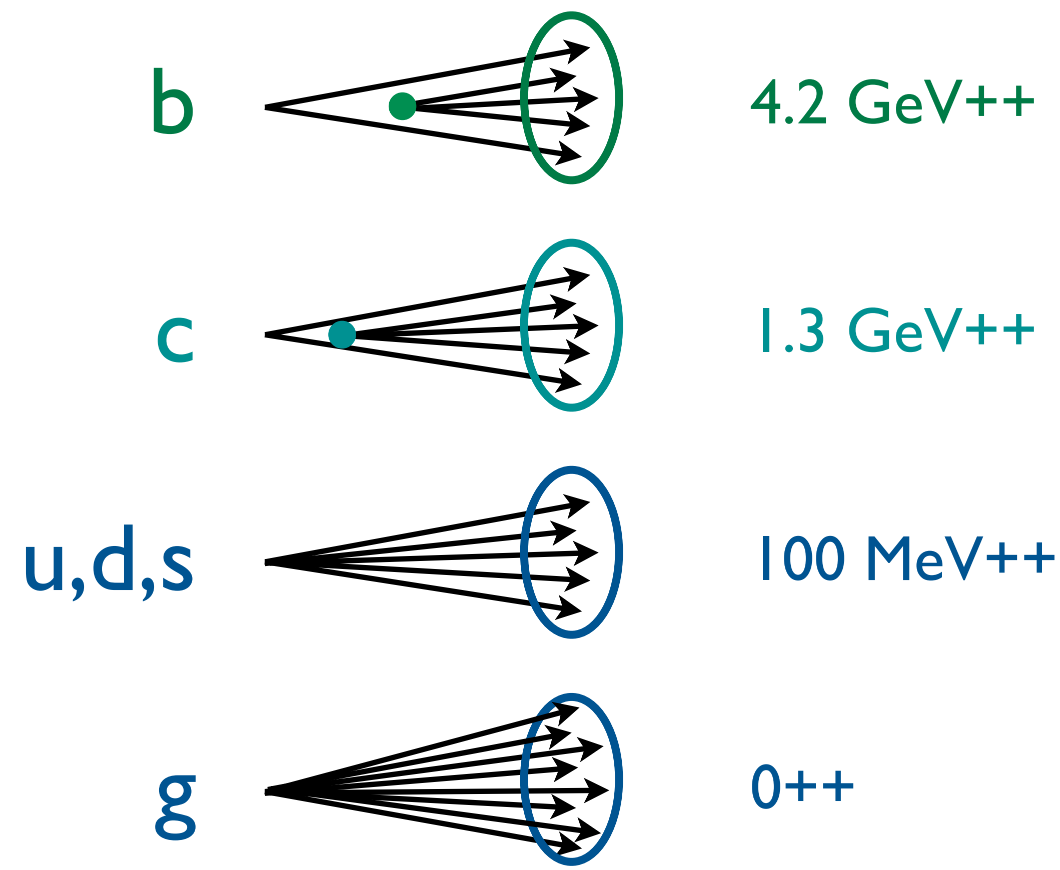
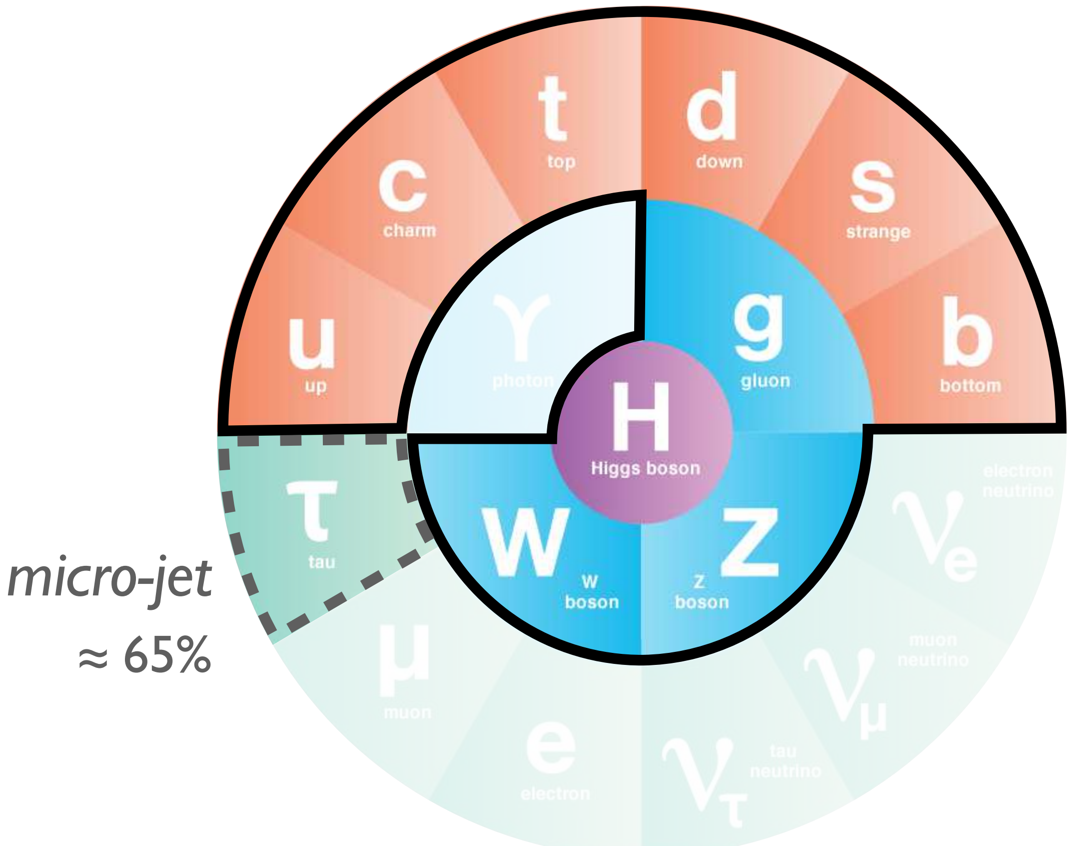
Date: 2010-07-18 11:05:54 CEST
ATLAS EXPERIMENT
Run: 302347
Event: 753275626
2016-06-18 18:41:48 CEST
CMS
Jet 1,
pt = 3.61 TeV
eta = 0.32
phi = 0.64
Jet 2,
pt = 3.38 TeV
eta = -0.56
phi = -2.49
CMS Experiment at LHC, CERN
Data recorded: Sat Apr 23 08:05:38 2011 EDT
Run/Event: 163332 / 196371106
ATLAS EXPERIMENT
CMS Experiment at LHC, CERN
Data recorded: Sat Aug 28 23:03:34 2010 EDT
Run/Event: 144089 / 671718071
Lumi section: 574
ATLAS EXPERIMENT
http://atlas.ch
Run: 209787
Event: 144100666
Date: 2012-09-05
Time: 03:57:49 UTC
Jet 0, pt: 205.1 GeV
Jet 1, pt: 70.0 GeV

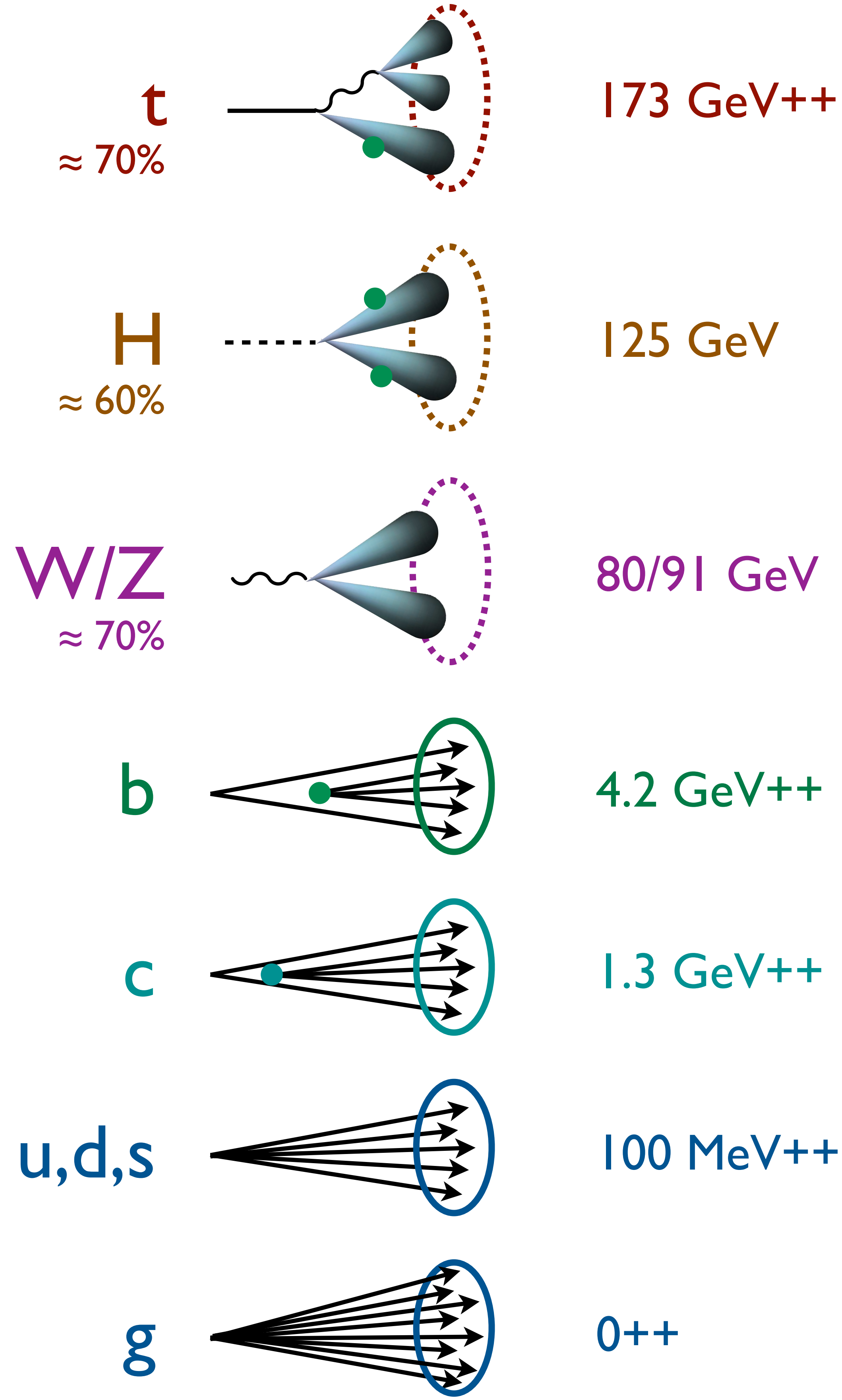


Jets from the Standard Model



++ = Mass from QCD Radiation





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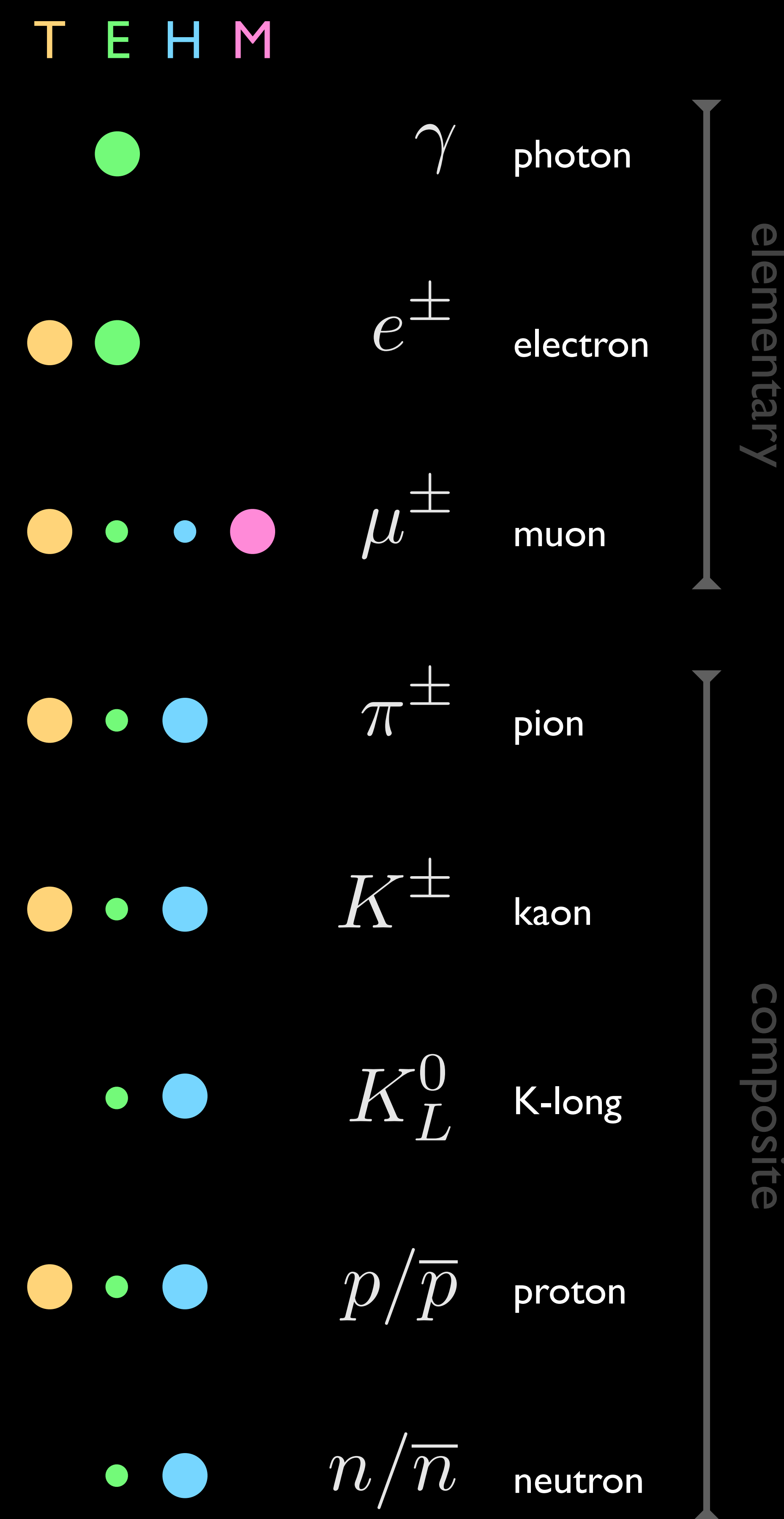
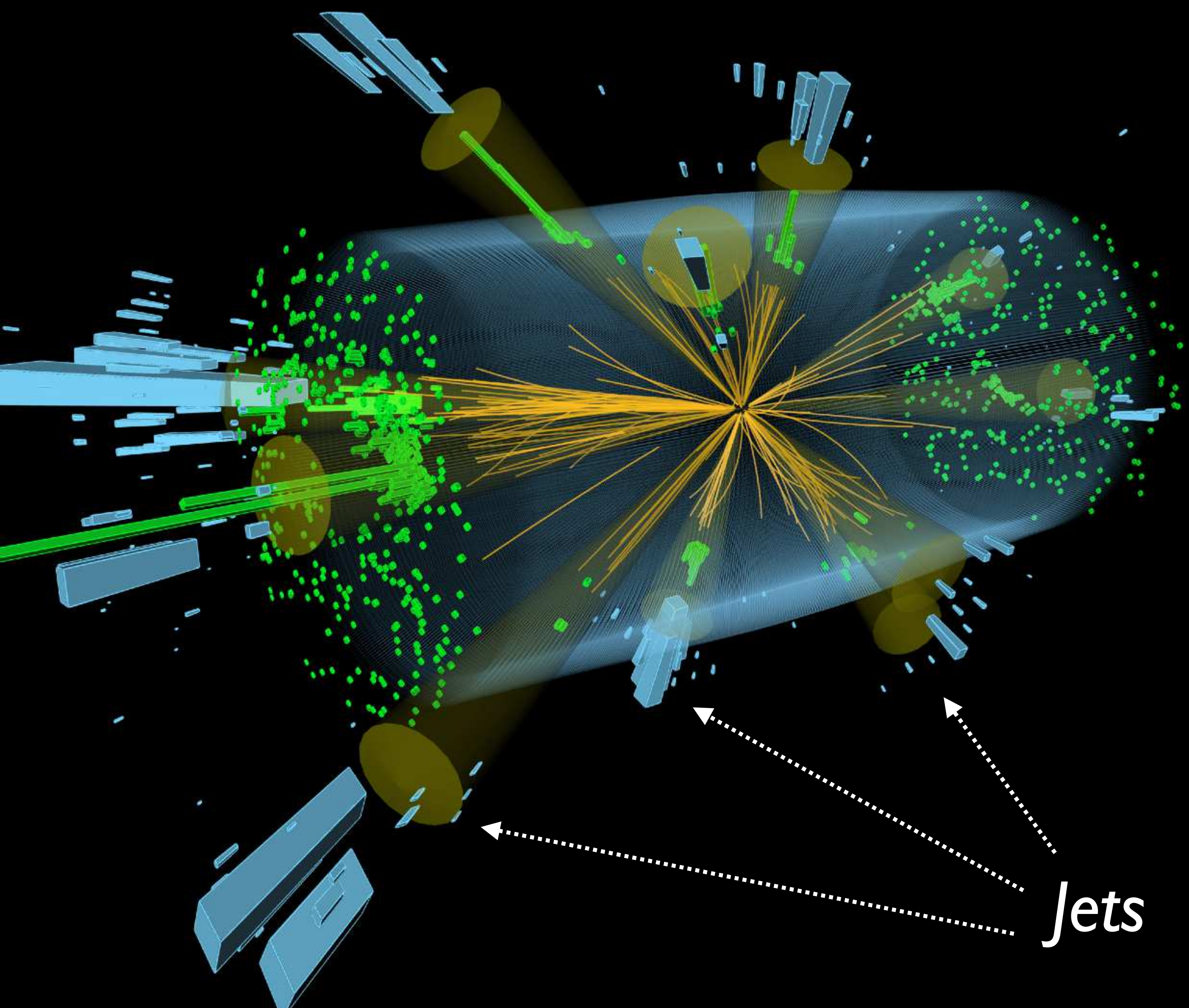

T E H M
γ photon
$e^{\pm}$ electron
$\mu^{\pm}$ muon
$\pi^{\pm}$ pion
$K^{\pm}$ kaon
K_L^0 K-long
$p/\overline{p}$ proton
$n/\overline{n}$ neutron
elementary
composite

Collider Event

Collection of points in (momentum) space



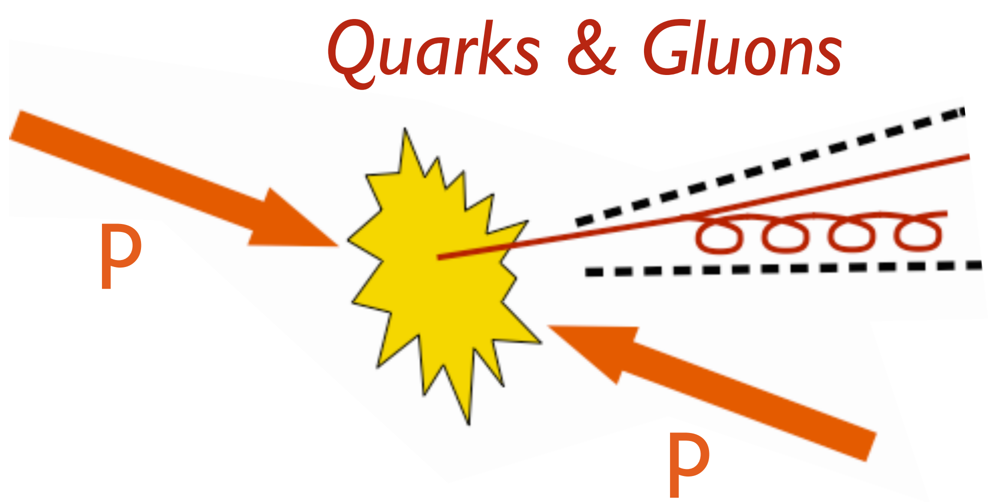
	T	E	H	M		
elementary		●			γ	photon
	●	●			$e^{\pm}$	electron
	●	•	•	●	$\mu^{\pm}$	muon
composite	●	•	●		$\pi^{\pm}$	pion
	●	•	●		$K^{\pm}$	kaon
		•	●		K_L^0	K-long
	●	•	●		$p/\overline{p}$	proton
		•	●		$n/\overline{n}$	neutron

Point Cloud

Collection of points in (position) space

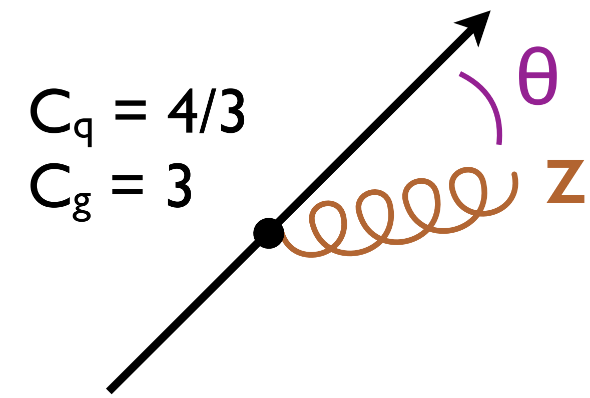
[Popular Science, 2013]

Dynamics of Jet Formation



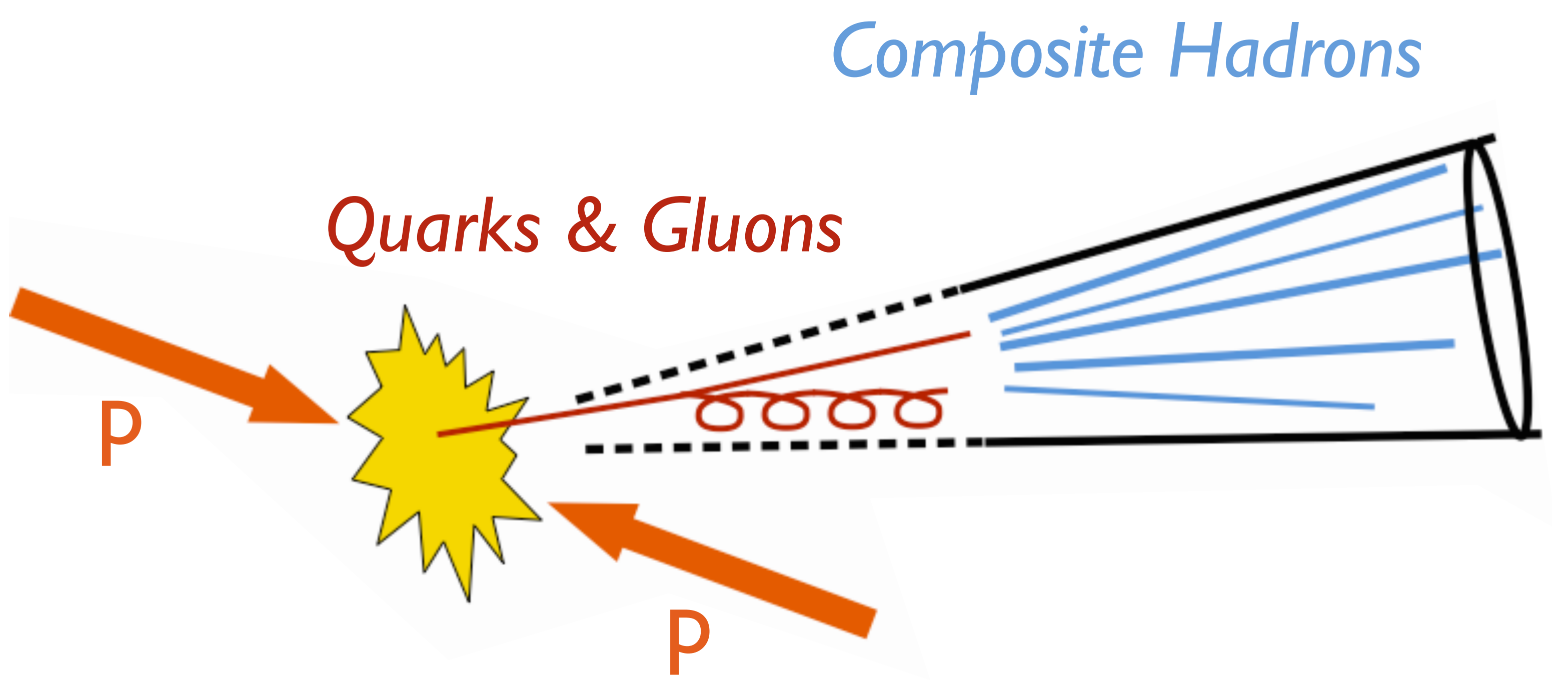
Altarelli-Parisi Splitting

Core prediction of QCD

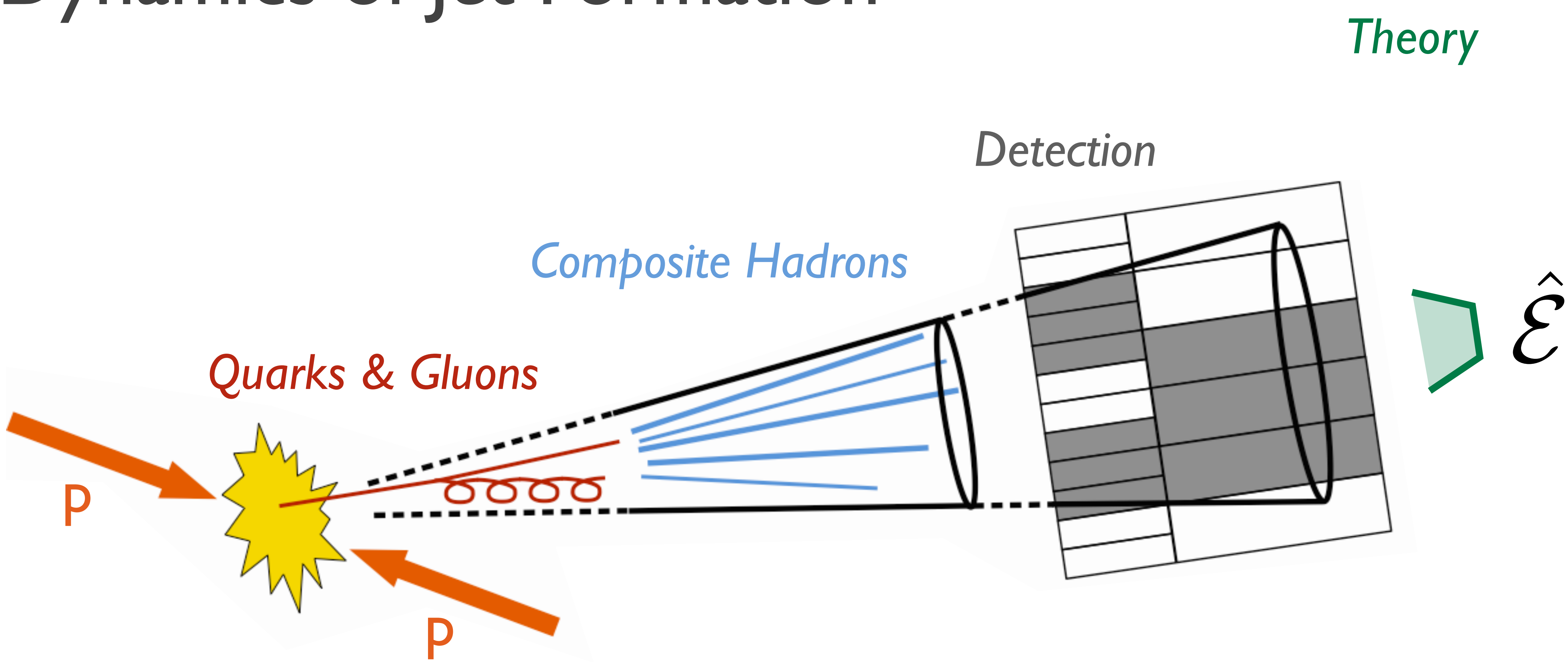


$$\mathrm{d}P_{i\to ig} \simeq \frac{2\alpha_s}{\pi} C_i \underbrace{\frac{\mathrm{d}\theta}{\theta}}_{\text{Collinear}} \underbrace{\frac{\mathrm{d}z}{z}}_{\text{Soft}}$$

Dynamics of Jet Formation



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

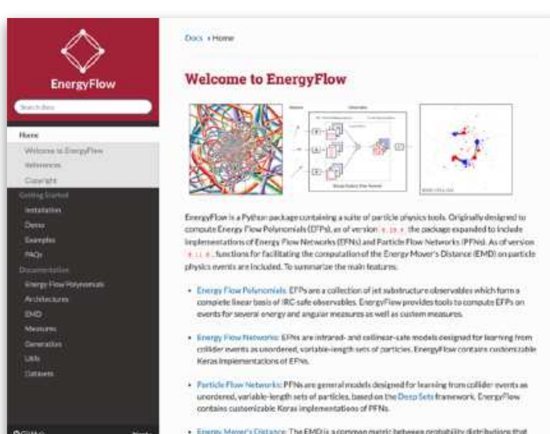
[Komiske, Metodiev, JDT, JHEP 2018]

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

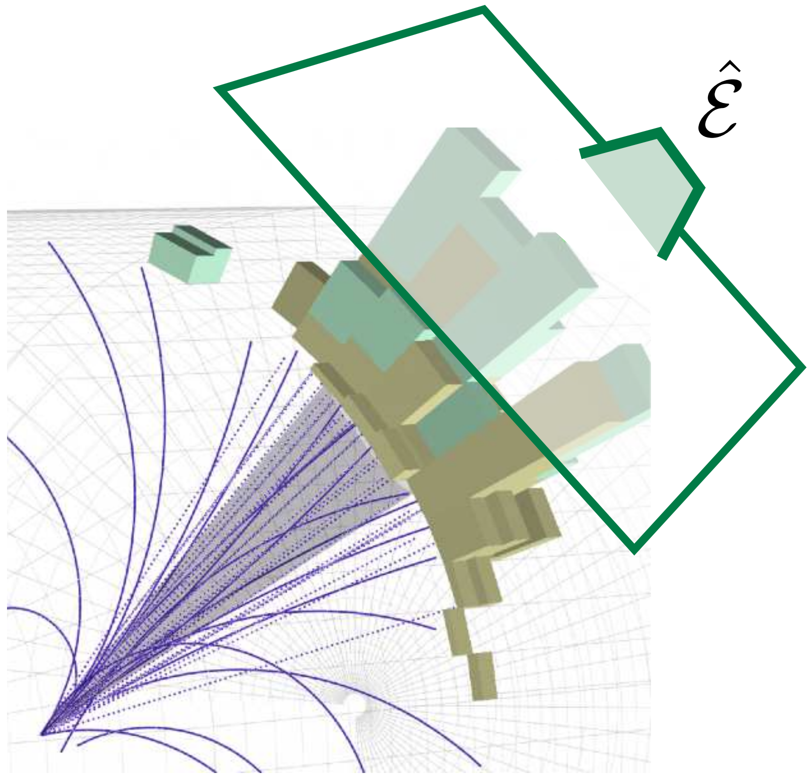
- Energy-Weighted Directions

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

Energy

Direction

(suppressing "unsafe" charge/flavor information)

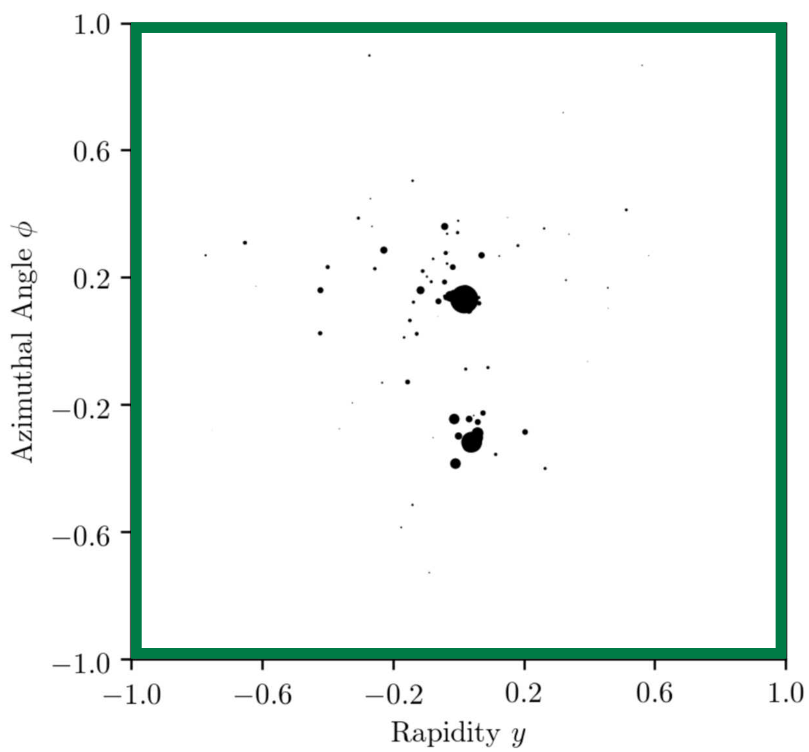


- Equivalently: Energy Density

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

Energy

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 $\{\mathcal{J}\}$

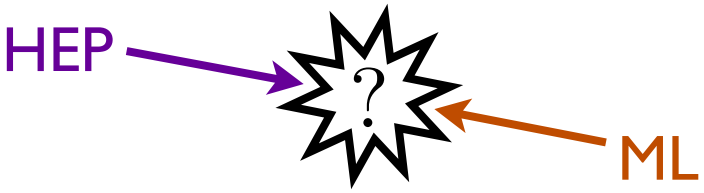
The Machine

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)

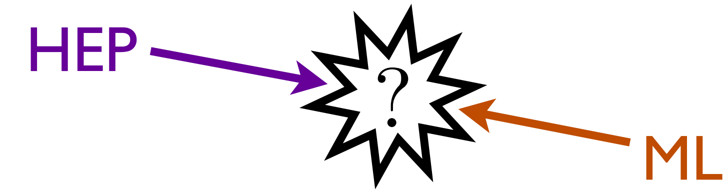
$$S(\mathcal{J}) = F(V_1, V_2, \ldots, V_\ell) \qquad V_a(\mathcal{J}) = \sum_{i \in \mathcal{J}} E_i \, \Phi_a(\hat{n}_i)$$

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

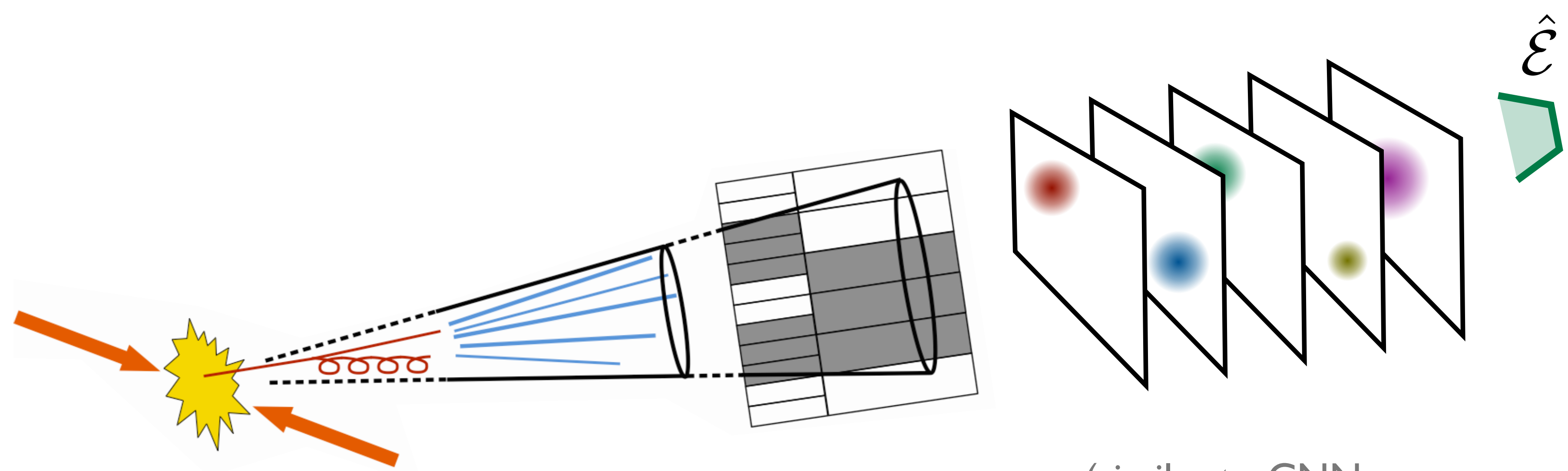


Architecture designed around symmetries and ***interpretability***

Latent space of dim ℓ

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

Easy to plot!

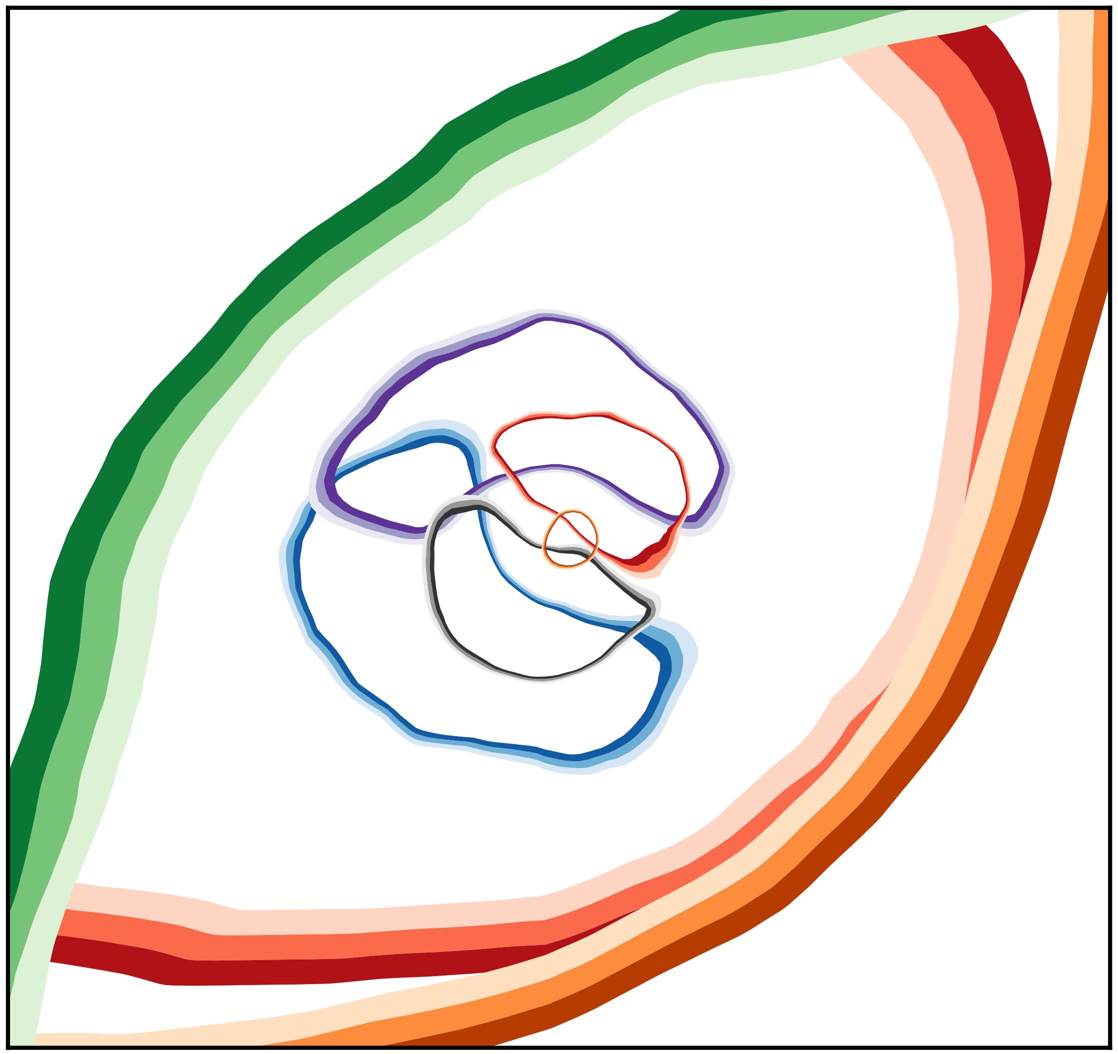


(similar to CNN filter activation)

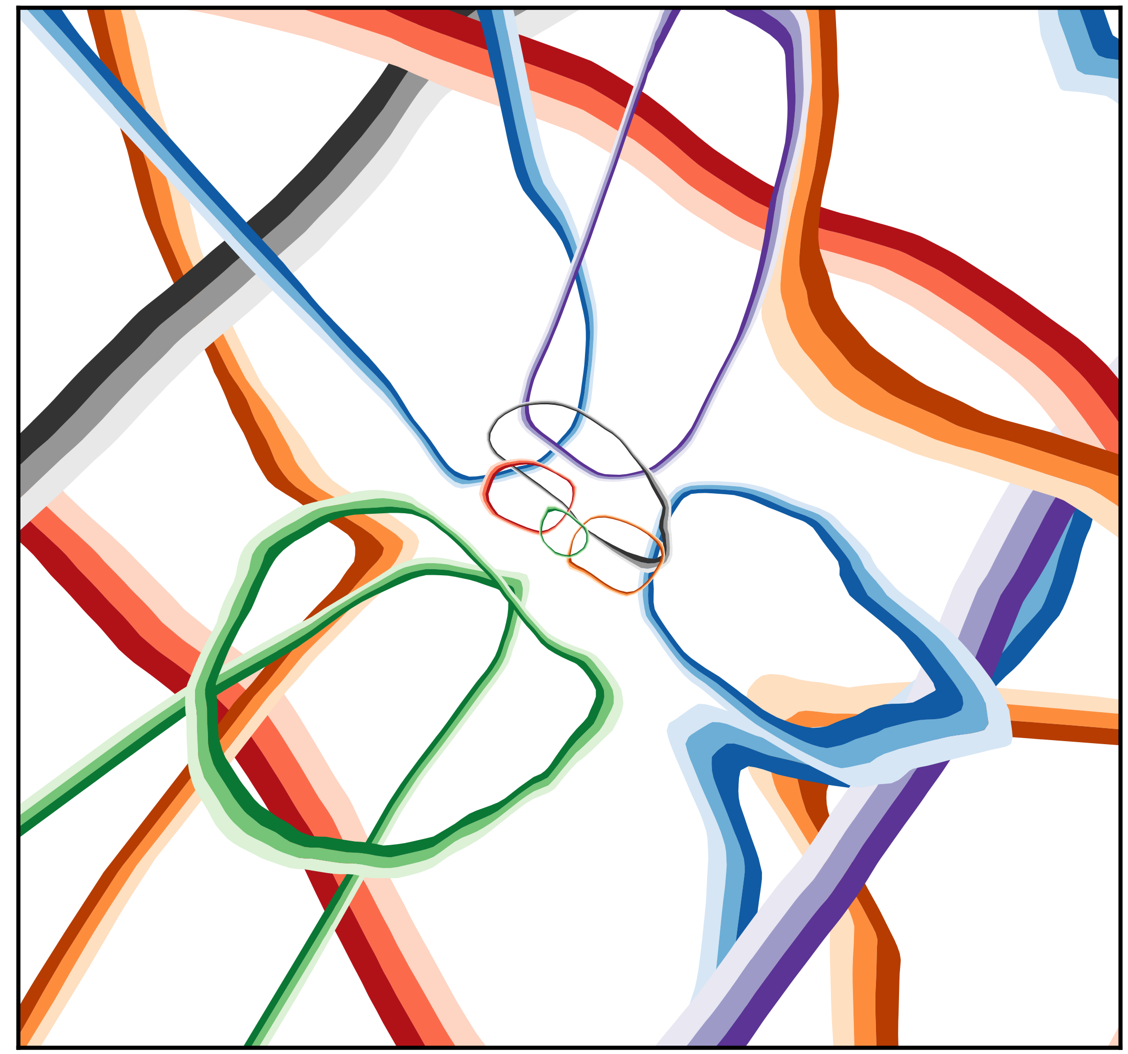
[Komiske, Metodiev, JDT, JHEP 2019; see also Komiske, Metodiev, JDT, JHEP 2018; code at energyflow.network; special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, NIPS 2017]

Psychedelic Network Visualization

Latent Dimension 8



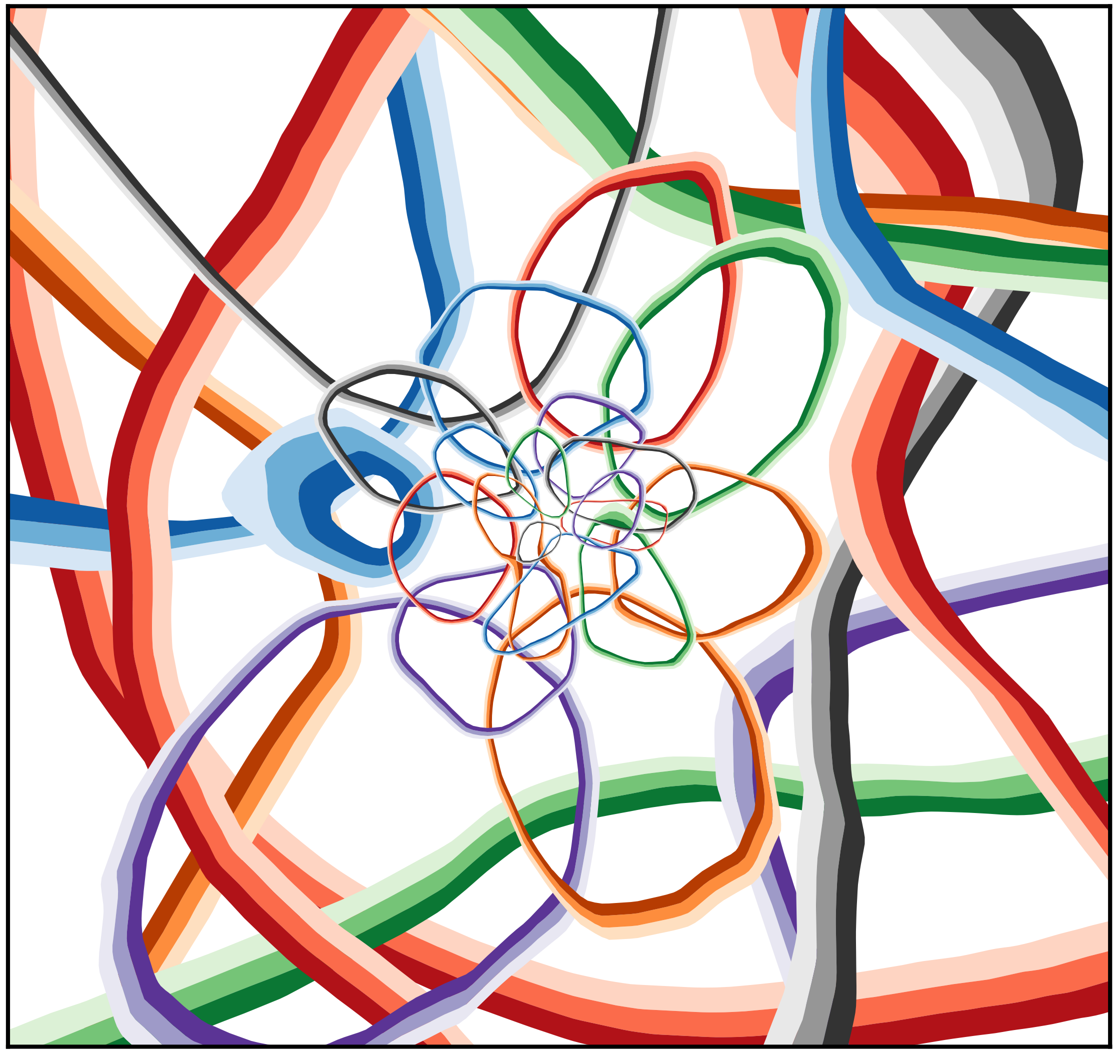
Latent Dimension 16



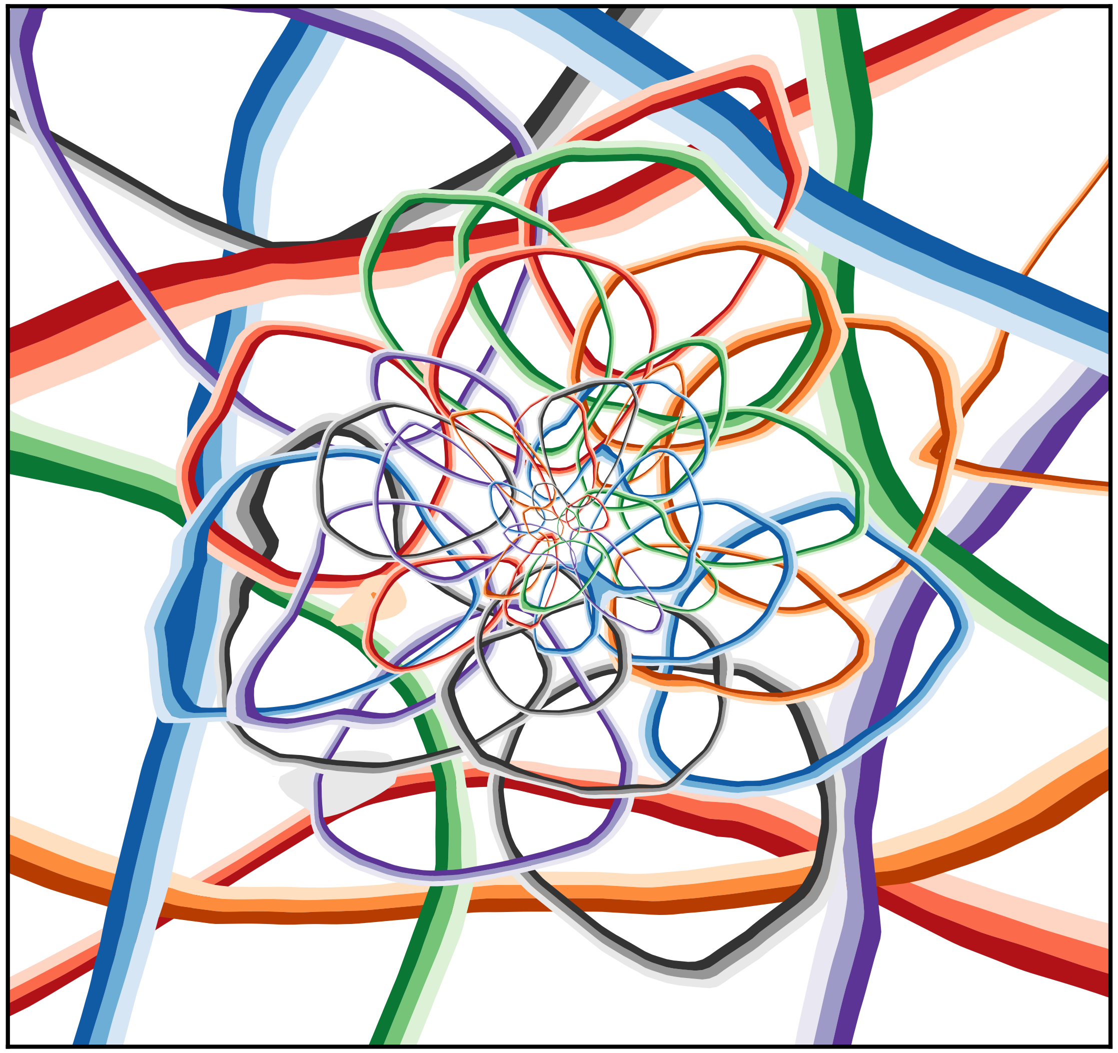
"Hello, World!" of Jets: Quark vs. Gluon

Psychedelic Network Visualization

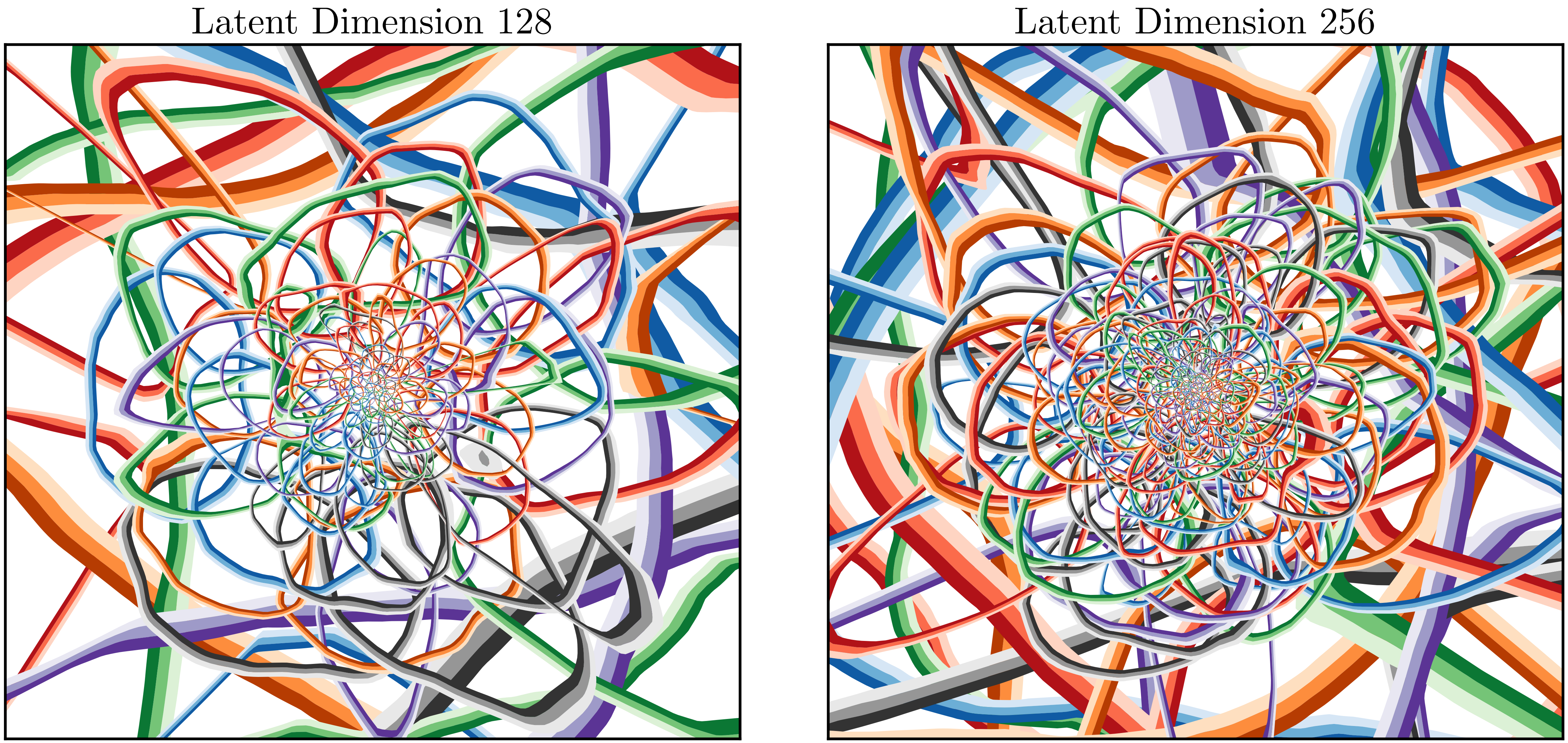
Latent Dimension 32



Latent Dimension 64

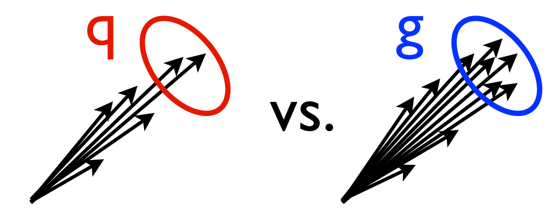


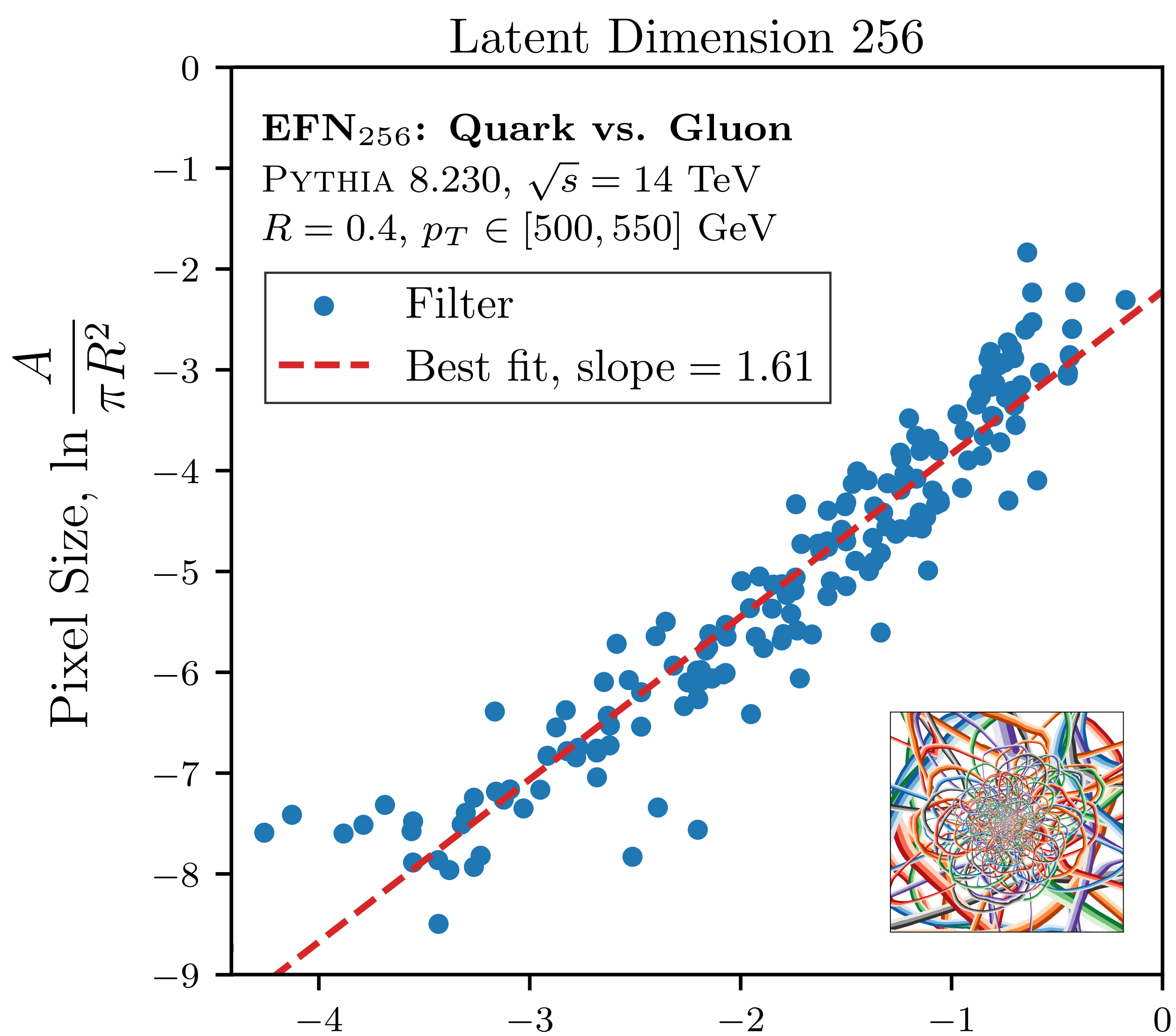
Psychedelic Network Visualization



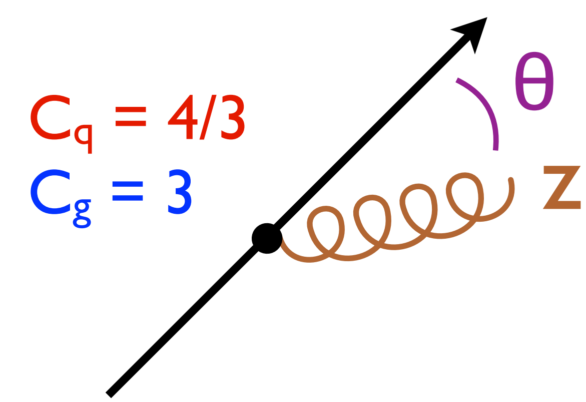
Fractal structure of the strong force!

Scaling of Strong Interactions





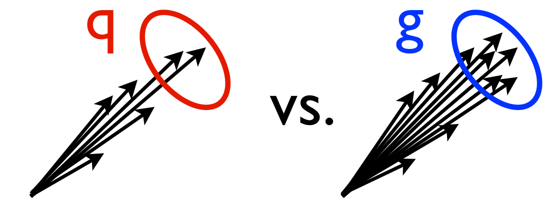
Radial Distance, $\ln \frac{\theta}{R}$

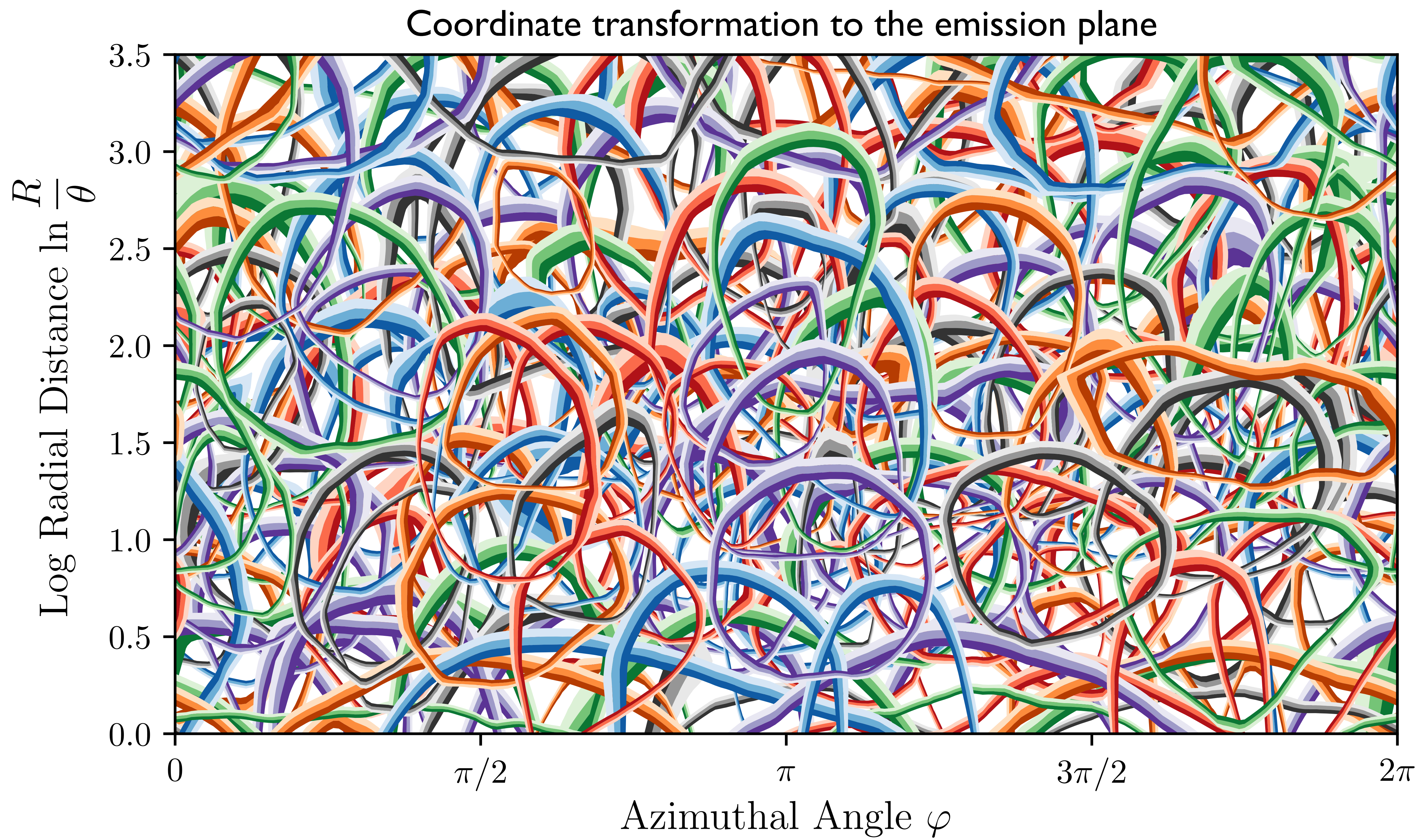


$$dP_{i \to ig} \simeq \frac{2\alpha_s}{\pi} C_i \underbrace{\frac{d\theta}{\theta}}_{\text{Collinear}} \underbrace{\frac{dz}{z}}_{\text{Soft}}$$

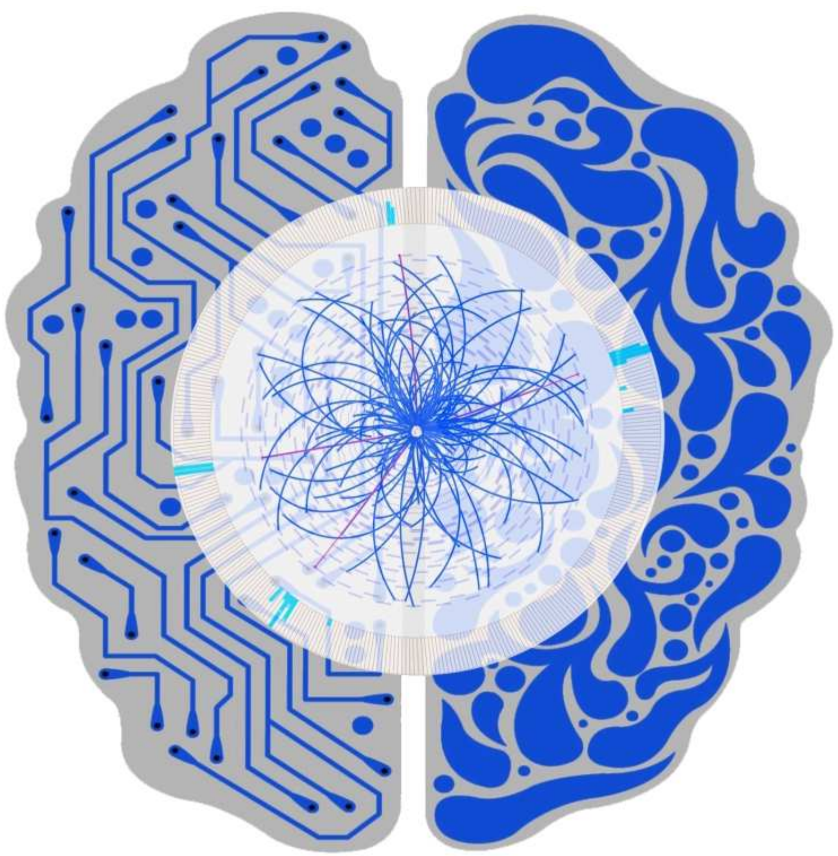
[Komiske, Metodiev, JDT, JHEP 2019]

Ready for the ICA?

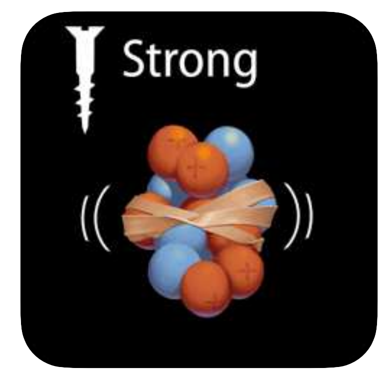




[Komiske, Metodiev, JDT, JHEP 2019; see also Dreyer, Salam, Soyez, JHEP 2018]



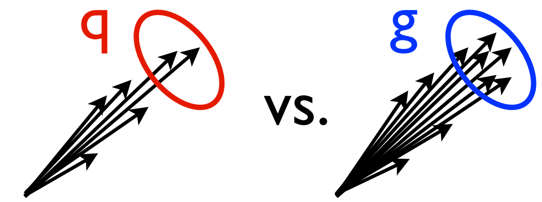
We taught a machine to "think" like a physicist…



…and it learned fractal structure of strong force!

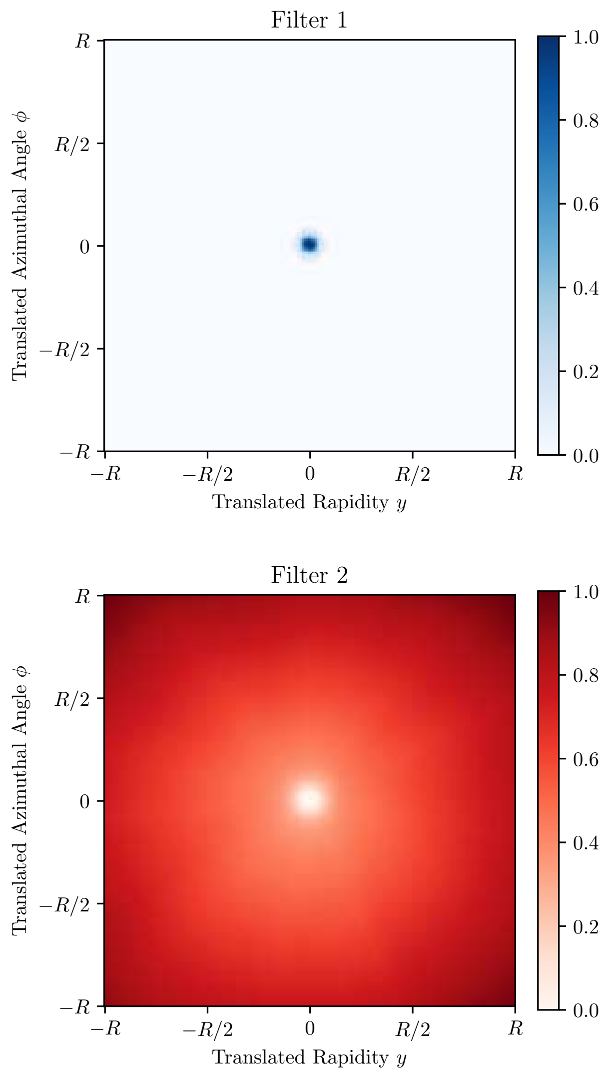
"Ok, but did you really learn something you didn't already know?"

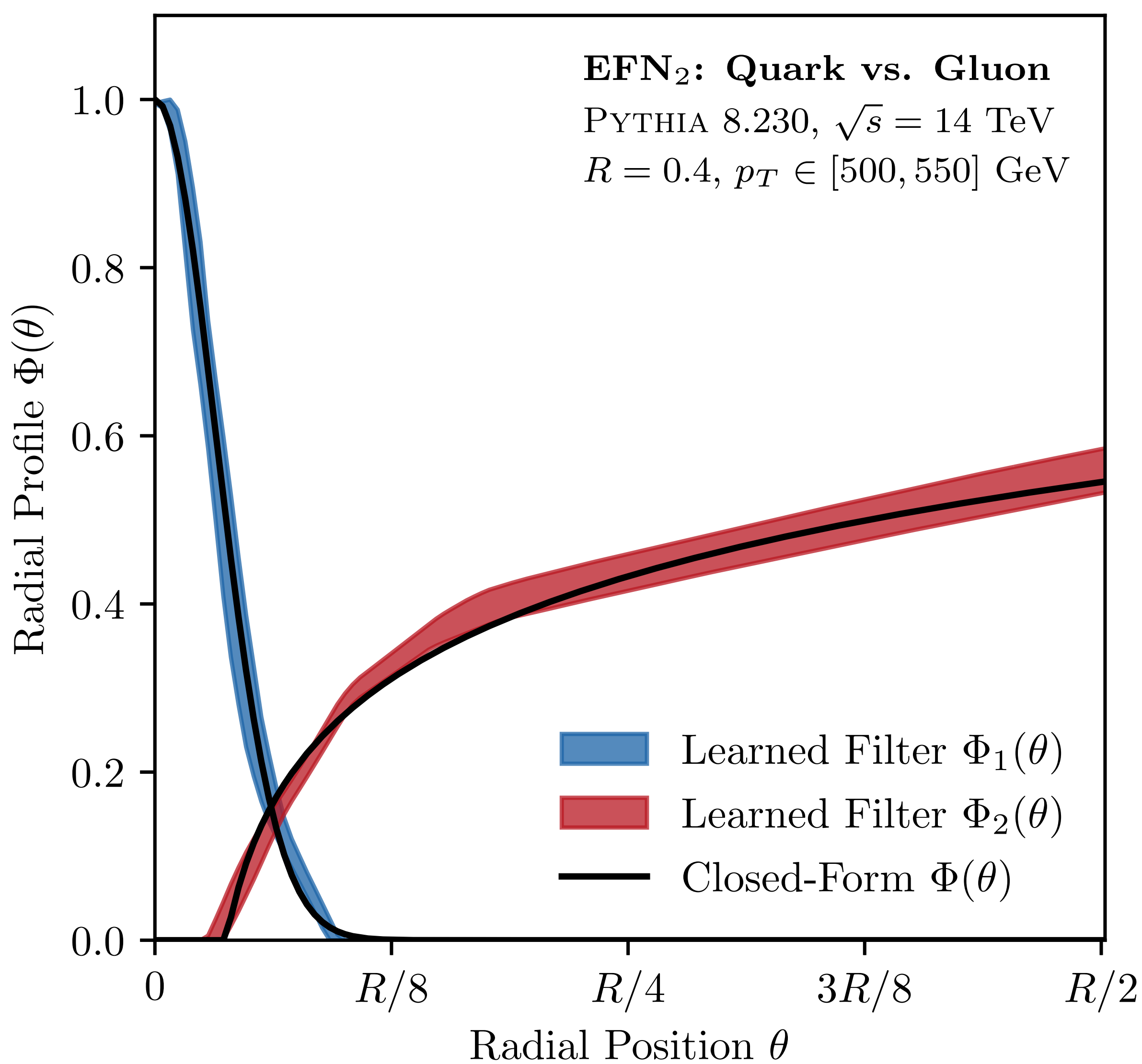
Learning from the Machine



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

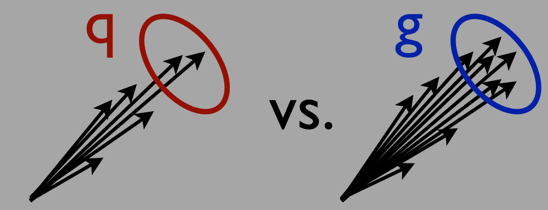
cf. Angularities:
$f(\theta) = \theta^\beta$





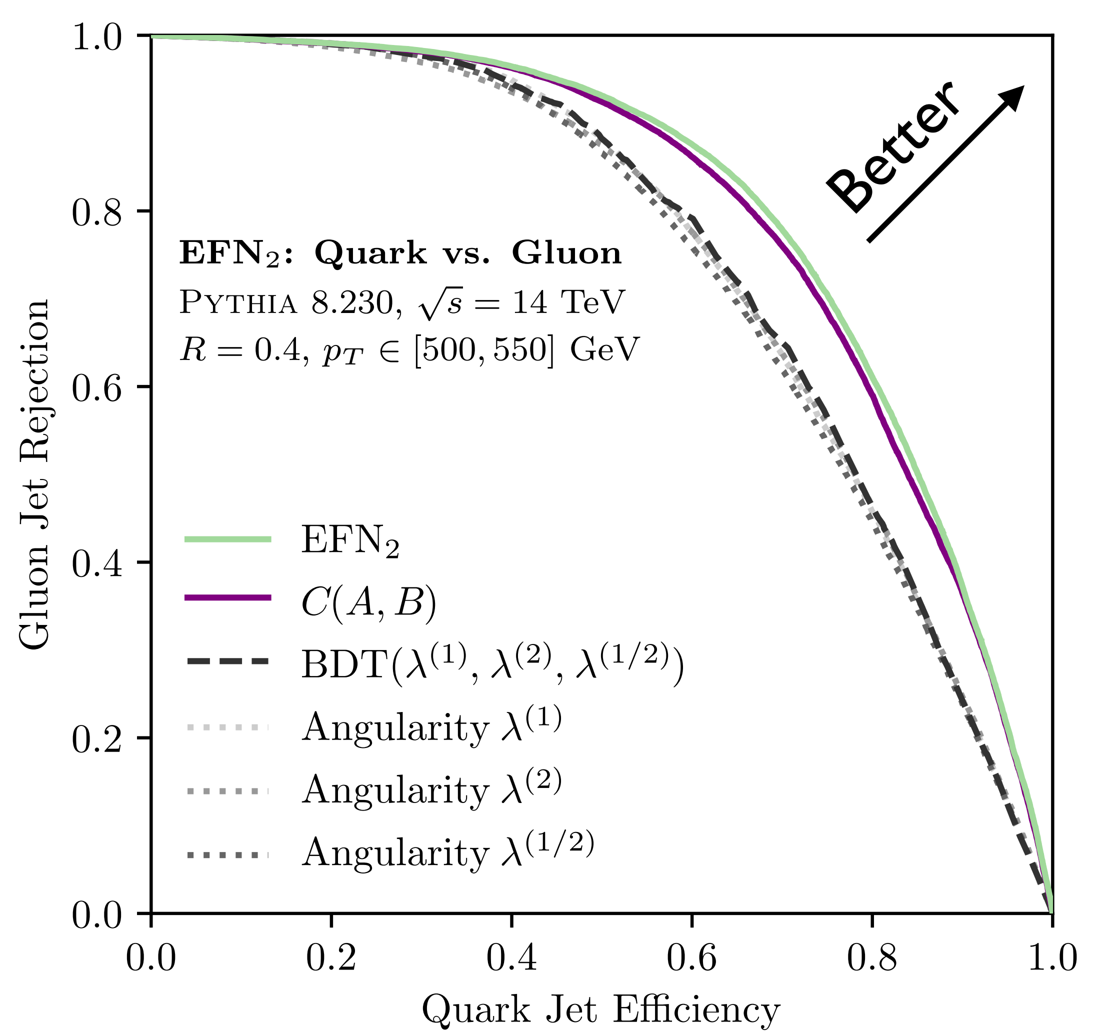
[Komiske, Metodiev, JDT, JHEP 2019;
cf. Larkoski, JDT, Waalewijn, JHEP 2014; using Berger, Kucs, Sterman, PRD 2003; Ellis, Vermilion, Walsh, Hornig, Lee, JHEP 2010]

Learning from the Machine



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

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



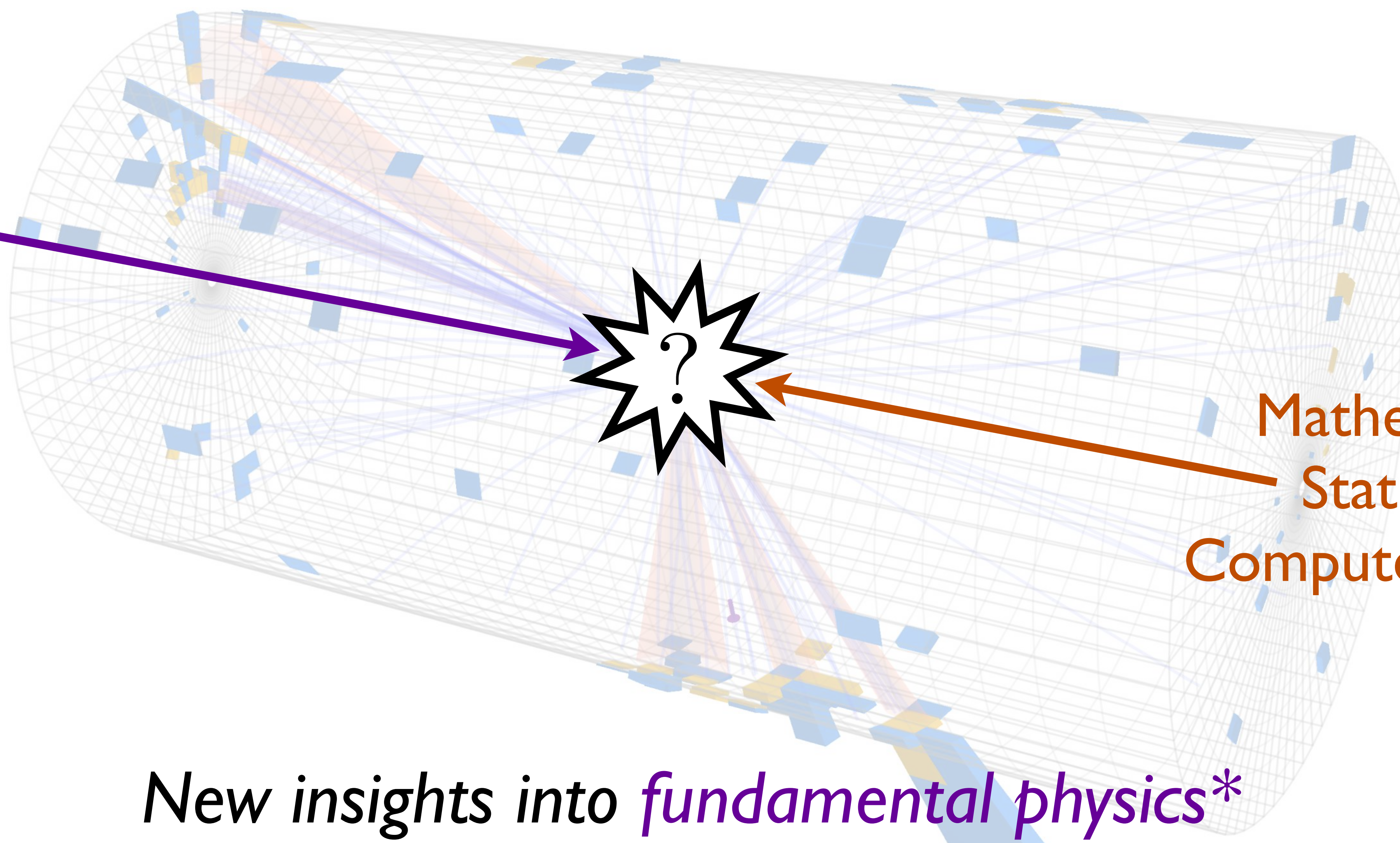
EFN outperformed a domain expert (i.e. me)

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]

“Collision Course”

Physical Sciences

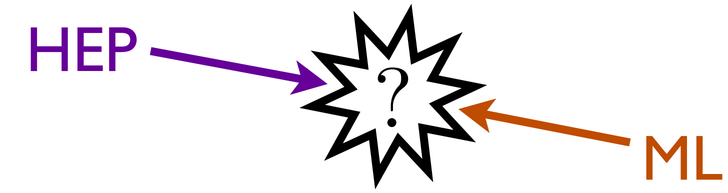


Mathematics, Statistics, Computer Science

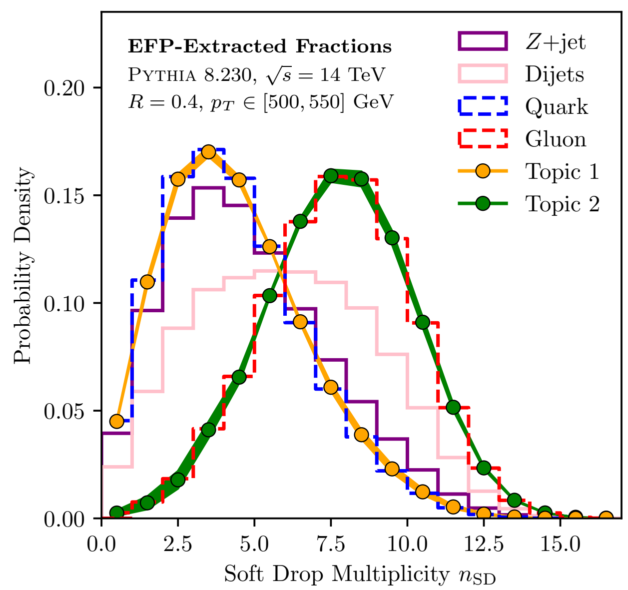
*New insights into fundamental physics**
*facilitated by advances in artificial intelligence**

(and vice versa!)

Recent Collisions

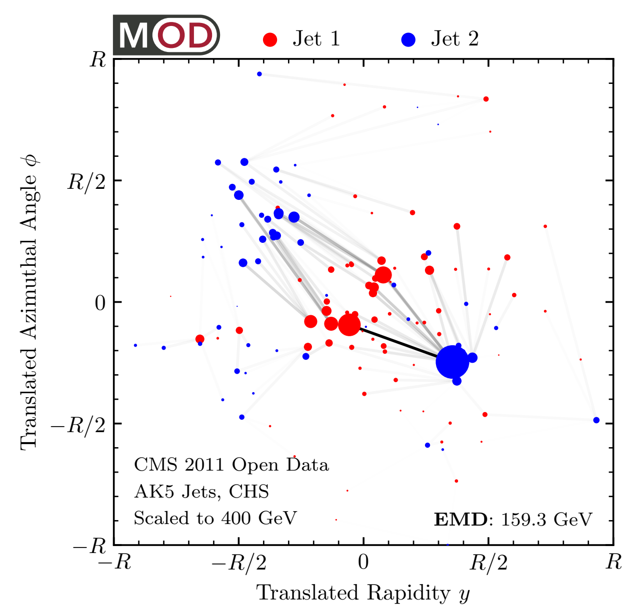


Quark/Gluon Definitions via Blind Source Separation



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

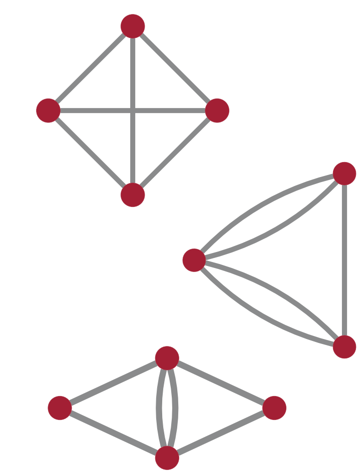
Half-Century of Collider Physics via Optimal Transport (!)



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

Kinematic Decomposition via Graph Theory

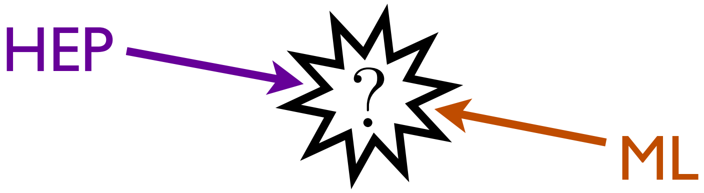
	Leafless Multigraphs	
Edges d	Connected A307317	All A307316
1	0	0
2	1	1
3	2	2
4	4	5
5	9	11
6	26	34
7	68	87
8	217	279
9	**718**	**897**
10	**2 553**	**3 129**
11	**9 574**	**11 458**
12	**38 005**	**44 576**
13	**157 306**	**181 071**
14	**679 682**	**770 237**
15	**3 047 699**	**3 407 332**
16	**14 150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



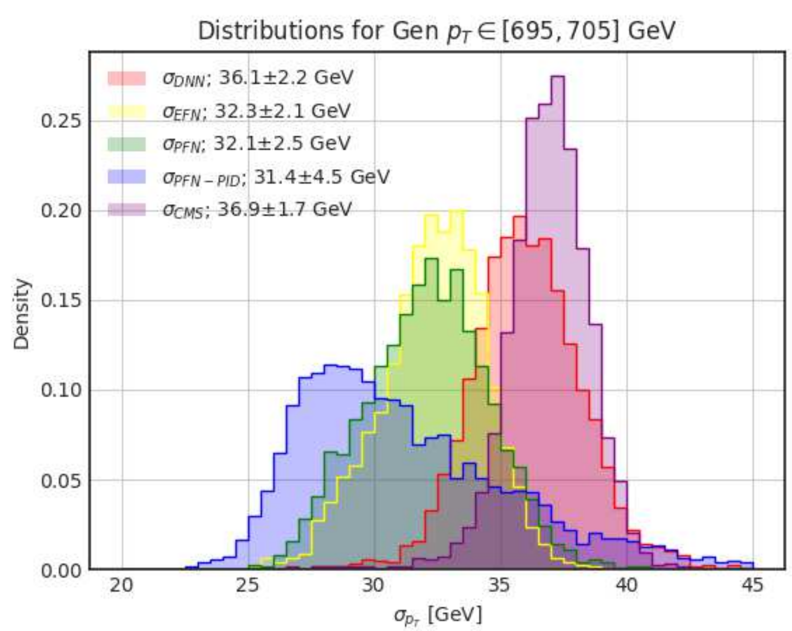
[Komiske, Metodiev, JDT, JHEP 2018, PRD 2020]

High Energy Physics ⇔ Mathematics, Statistics & Computer Science

Ongoing Collisions

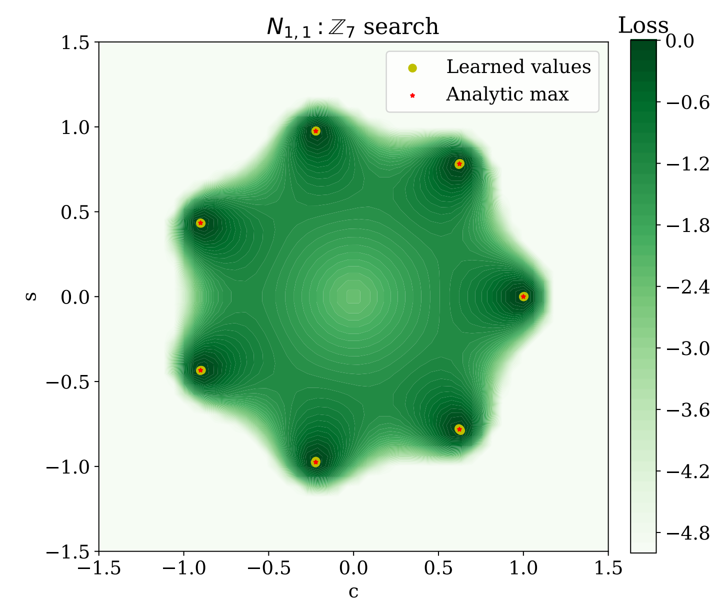


Frequentist Jet Calibration
via Gaussian Ansatz



[Nachman, Gambhir, JDT, in progress]

Symmetry Discovery
via Adversarial Learning

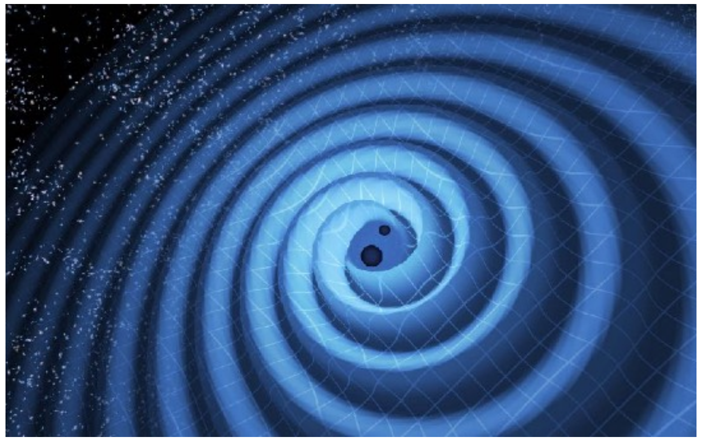


[Desai, Nachman, JDT, NeurIPS 2021 ML4PS]

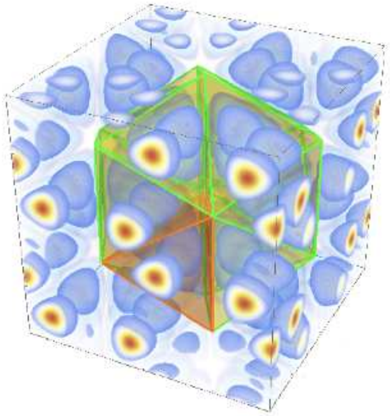
High Energy Physics ⇔ *Mathematics, Statistics & Computer Science*

Artificial Intelligence ⇔ *Fundamental Interactions*

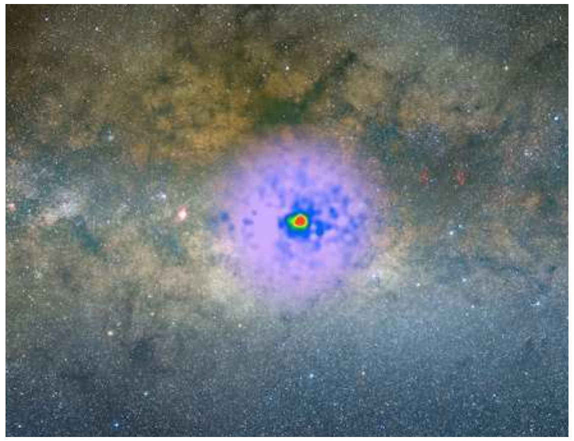
Gravitational Waves



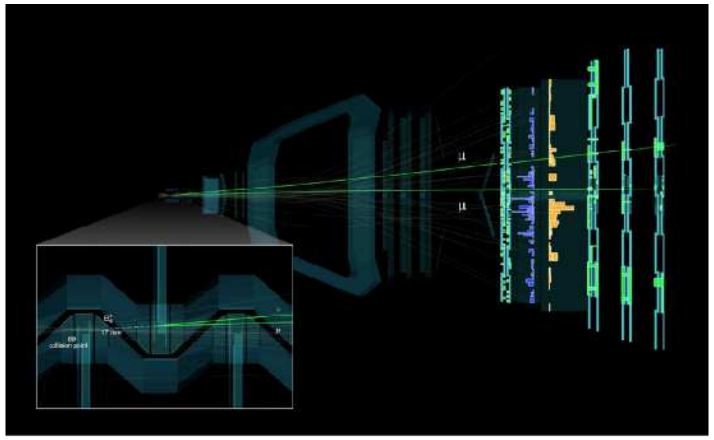
Nuclear Physics



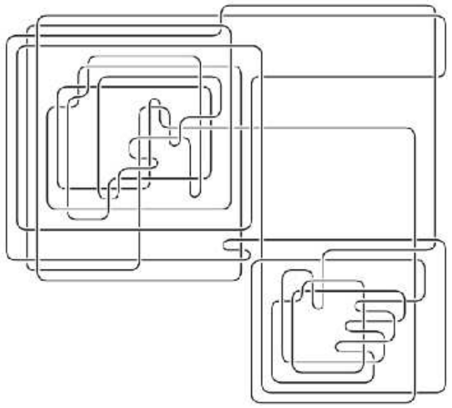
Astrophysics



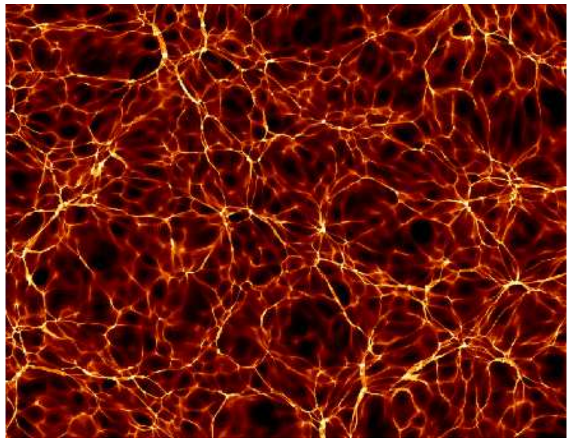
Particle Colliders



Mathematical Physics



Dark Matter



…

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

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http://iaifi.org/