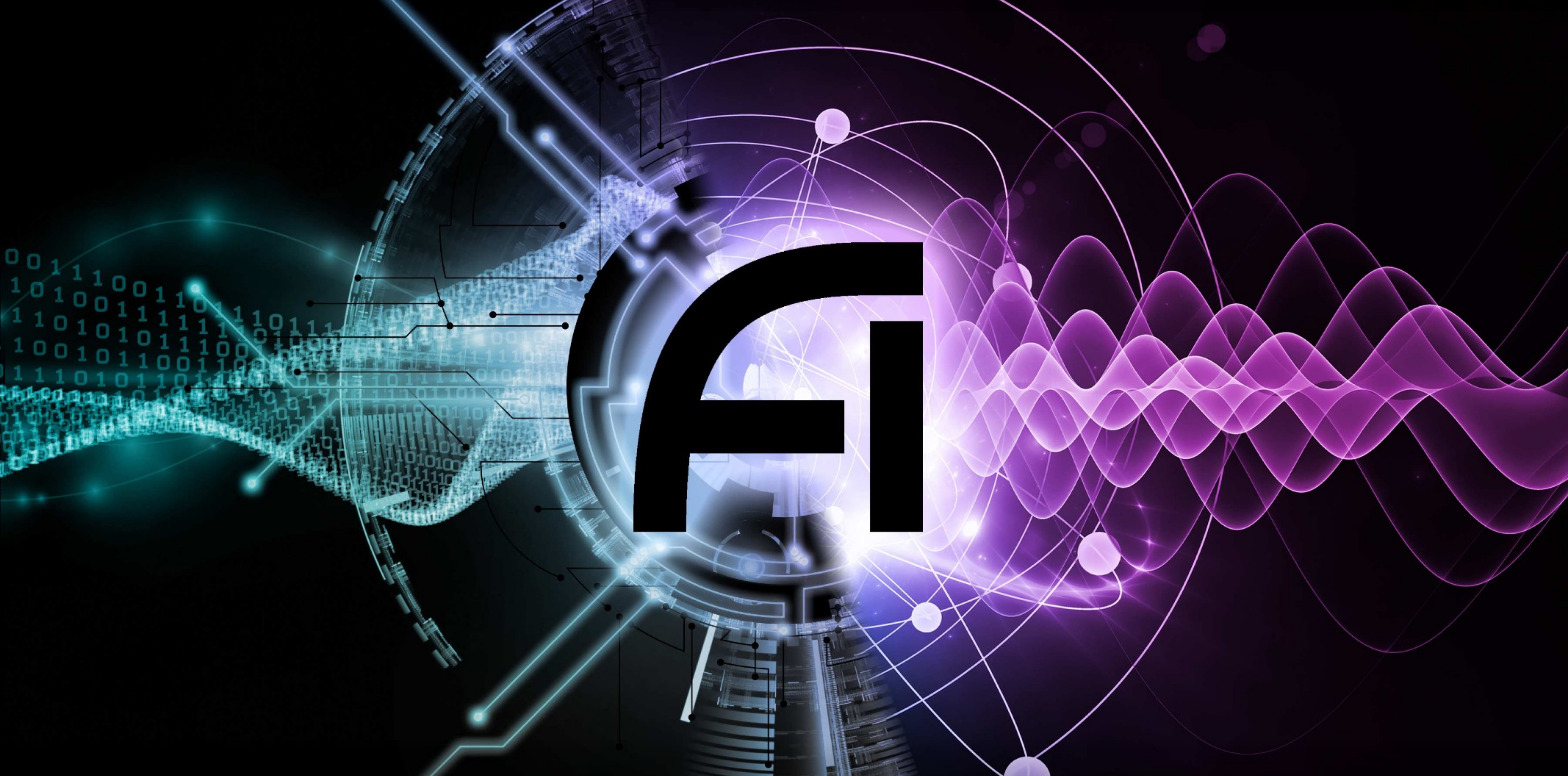
Particle Physics through the Lens of Machine Learning

Jesse Thaler

Brown Physics Colloquium — November 7, 2022

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI /aɪ-faɪ/ iaifi.org)



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

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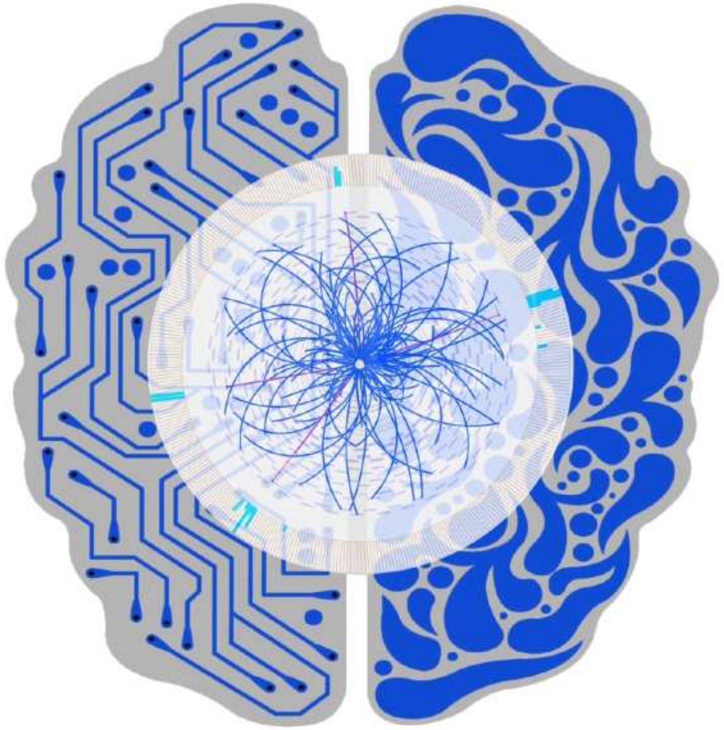


Infuse physics intelligence into artificial intelligence

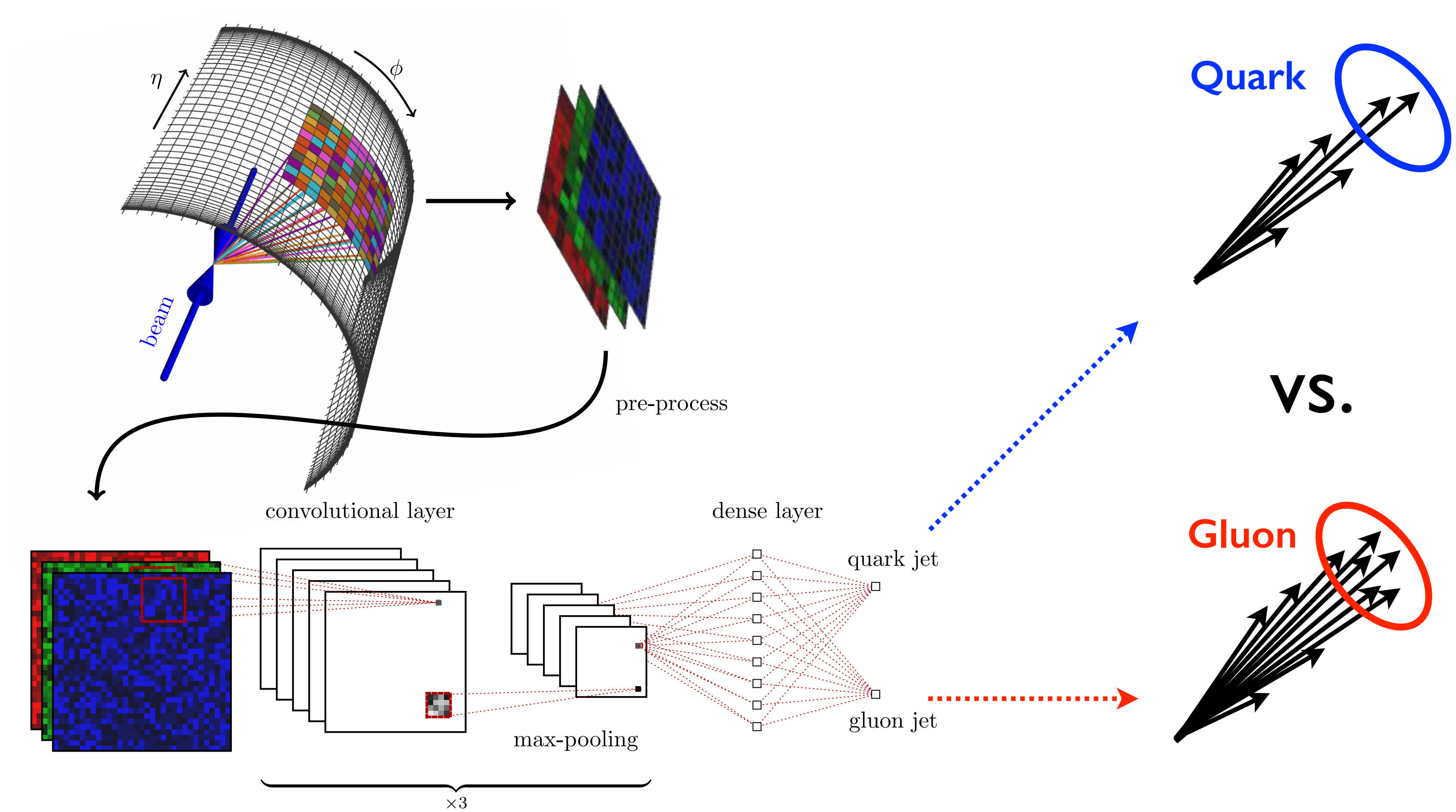
Machine learning that incorporates
first principles, best practices, and domain knowledge
from fundamental physics

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

Weak Supervision for the Strong Force

An IAIFI origin story: Patrick and Eric come to my office at MIT…

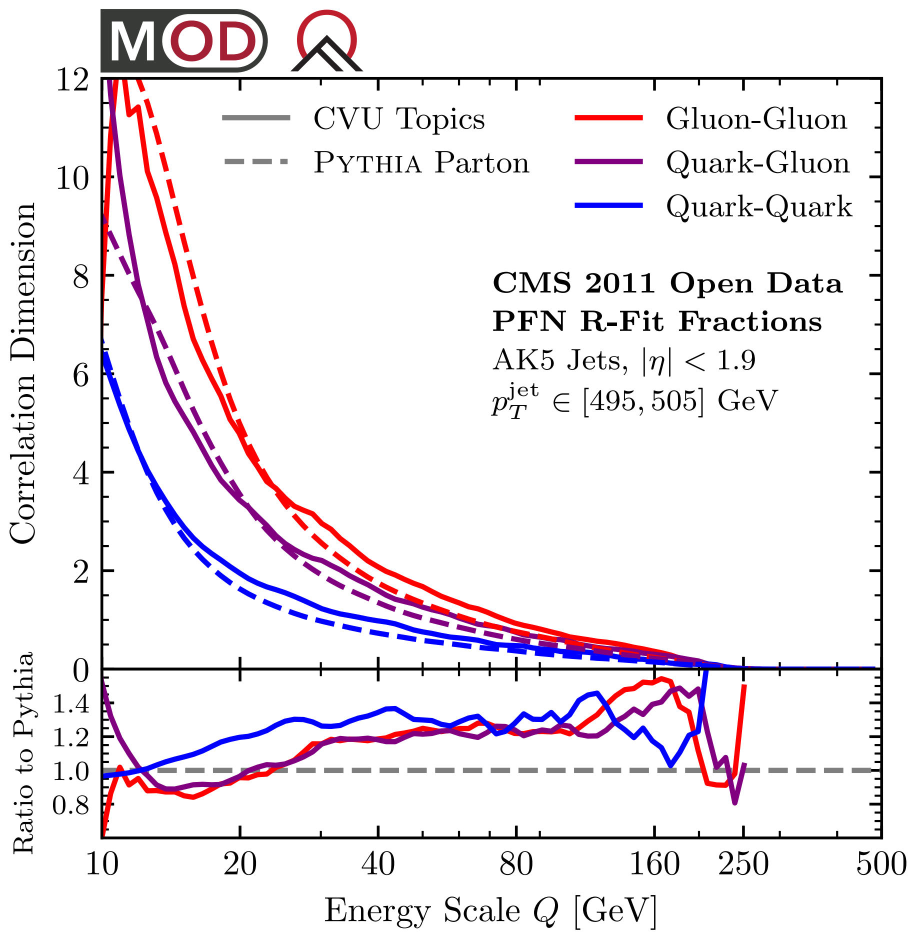
Fully supervised learning:



"What do you mean by quarks and gluons?"


[Komiske, Metodiev, Schwartz, JHEP 2017]

Weak Supervision for the Strong Force



Five years later,
I finally know an answer!

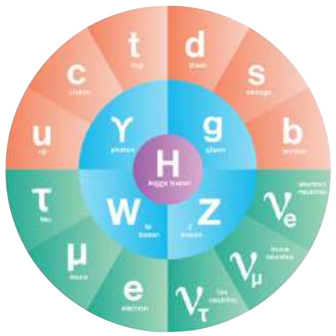
Required weak supervision, topic modeling, permutation-invariant networks, simulation-based inference, optimal transport, …

[Komiske, Kryhin, JDT, PRD 2022]

"What do you mean by quarks and gluons?"

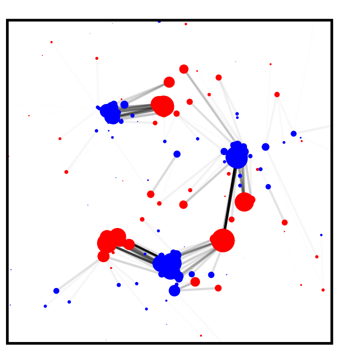
[Komiske, Metodiev, Schwartz, JHEP 2017]

Outline

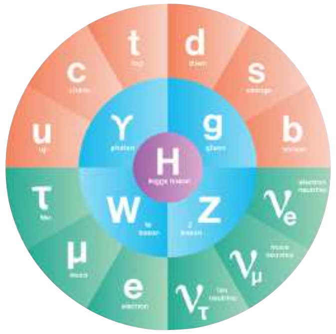


2017: A Quark/Gluon Conundrum

2018: Leveraging Weak Supervision



2019-2022: The Strong Force Revisited



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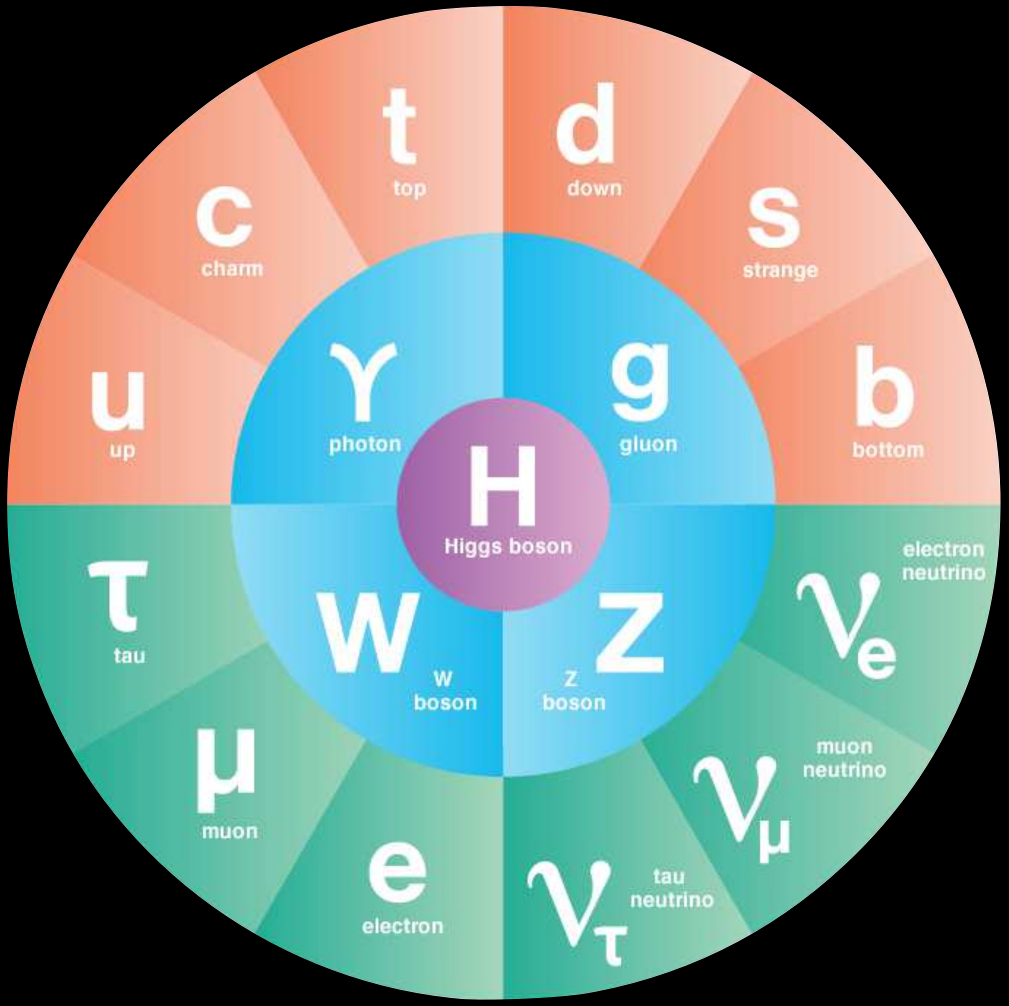
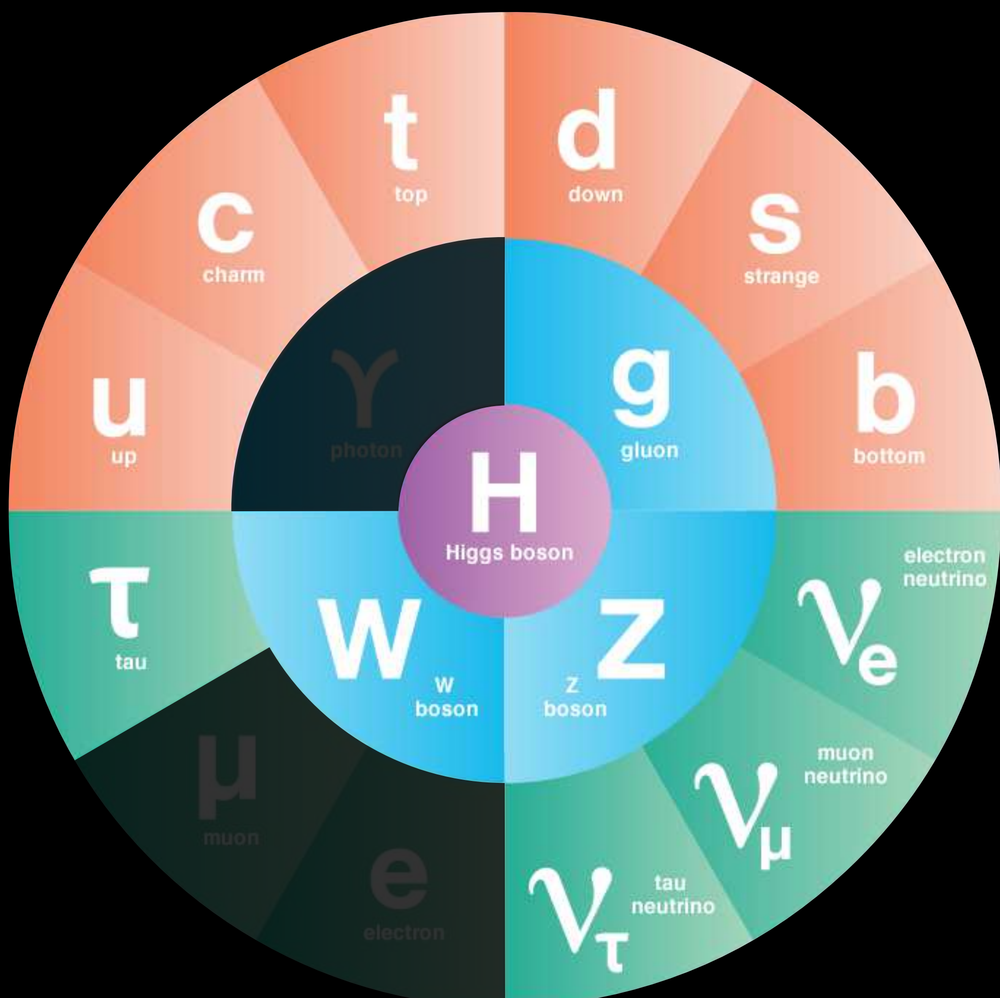
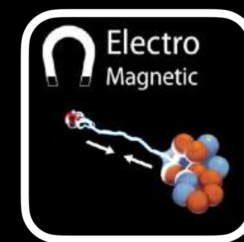
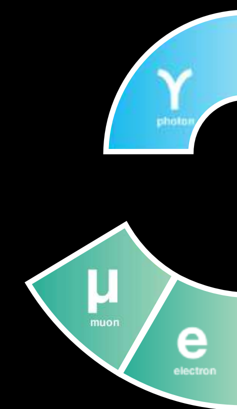
Particle Physics 101



Particle Physics 101







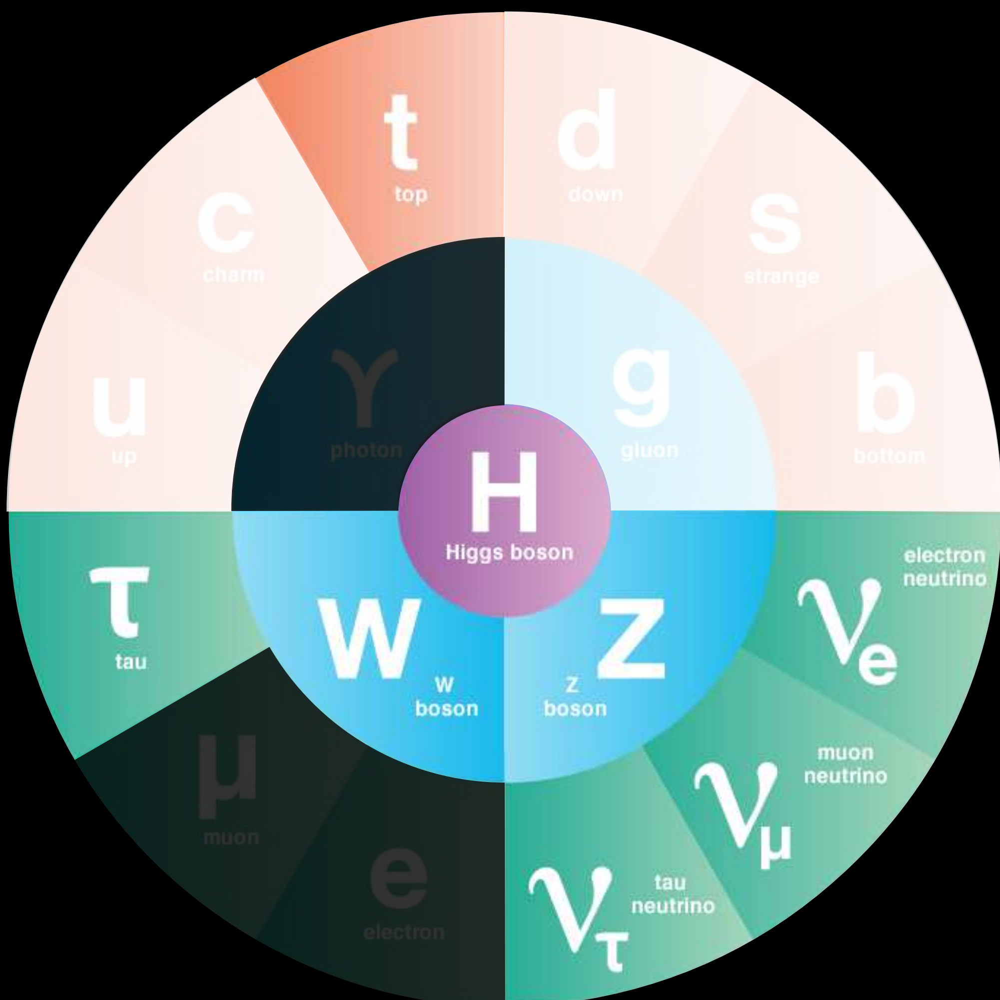
γ photon

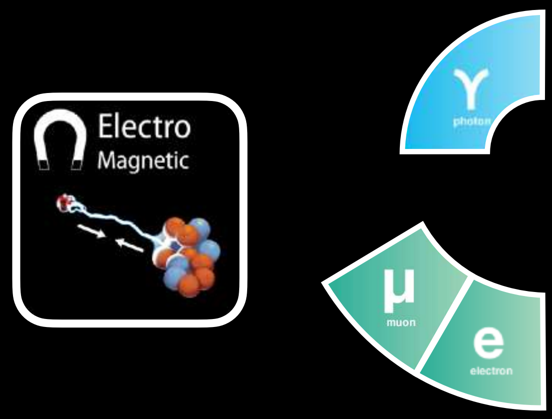
$e^{\pm}$ electron

$\mu^{\pm}$ muon

elementary

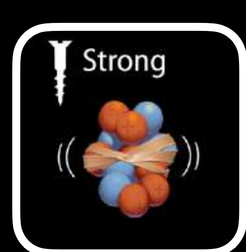
Particle Physics 101

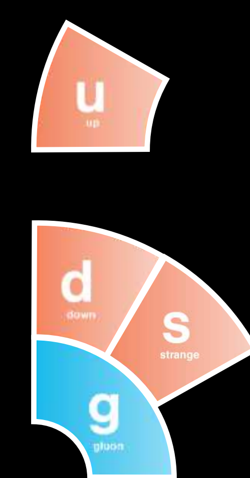




Strong Force
⇒ Confinement

Quarks
&
Gluons





elementary

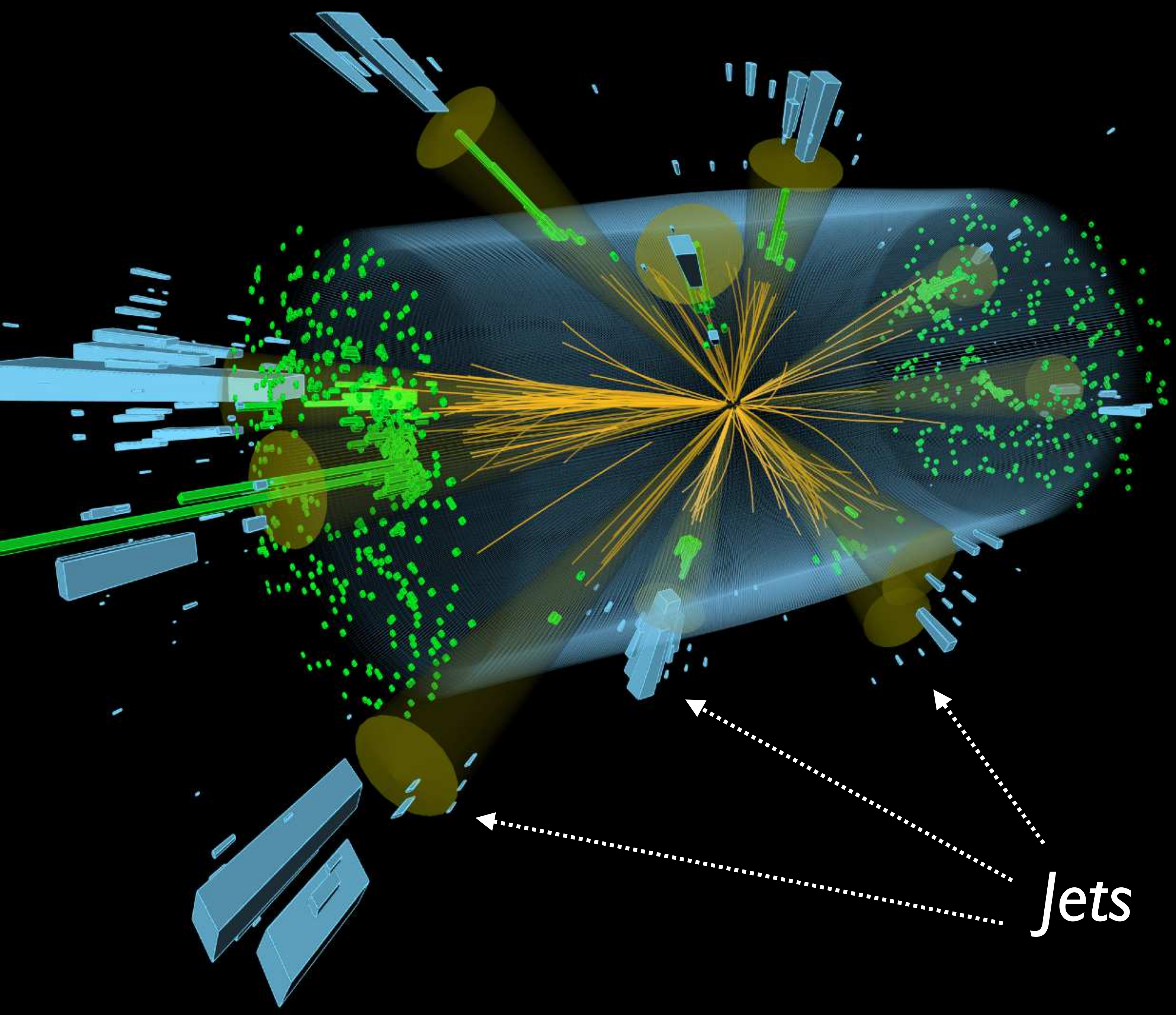
γ	photon
$e^{\pm}$	electron
$\mu^{\pm}$	muon

composite

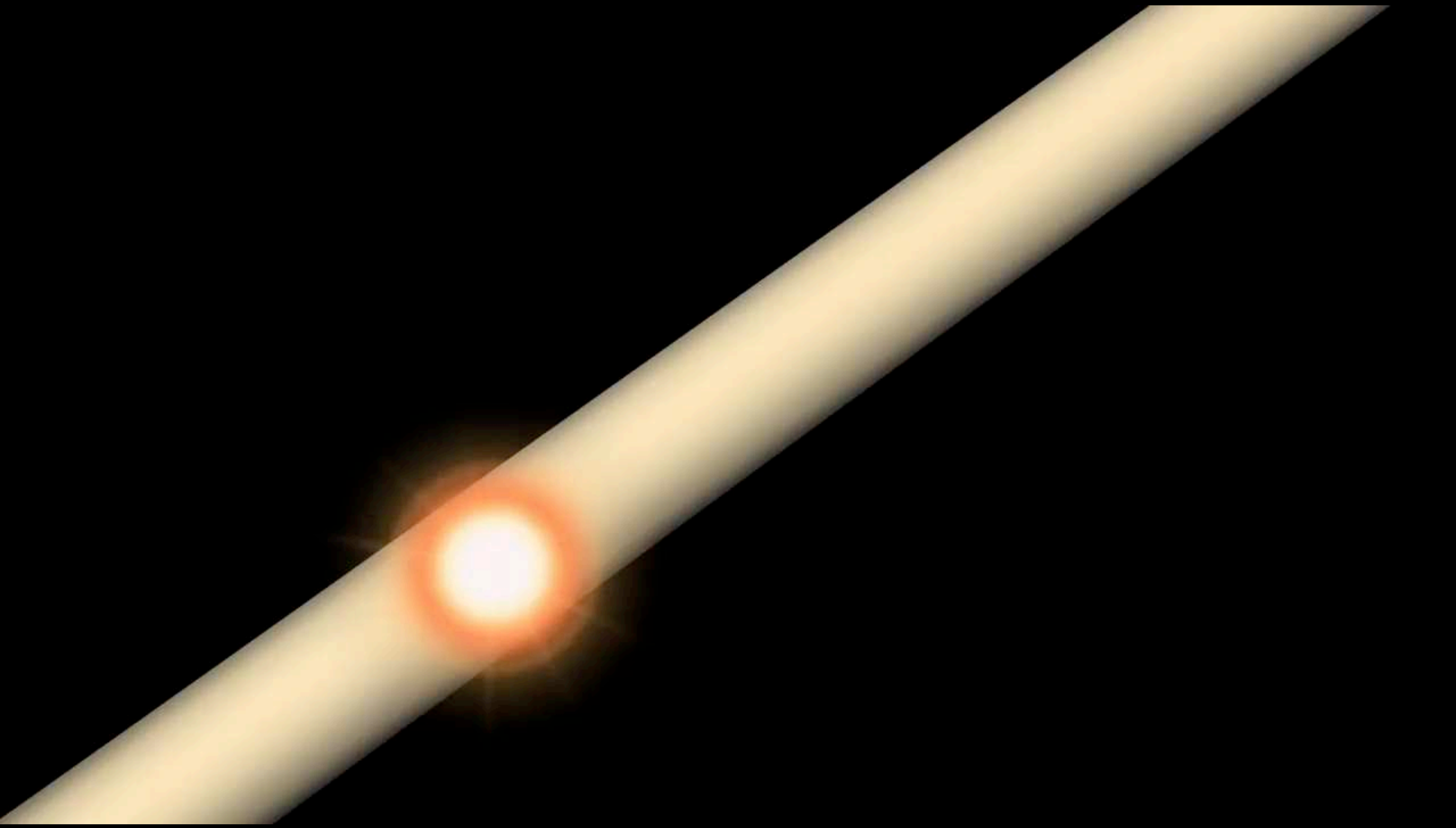
$\pi^{\pm}$	pion
$K^{\pm}$	kaon
K_L^0	K-long
$p/\overline{p}$	proton
$n/\overline{n}$	neutron

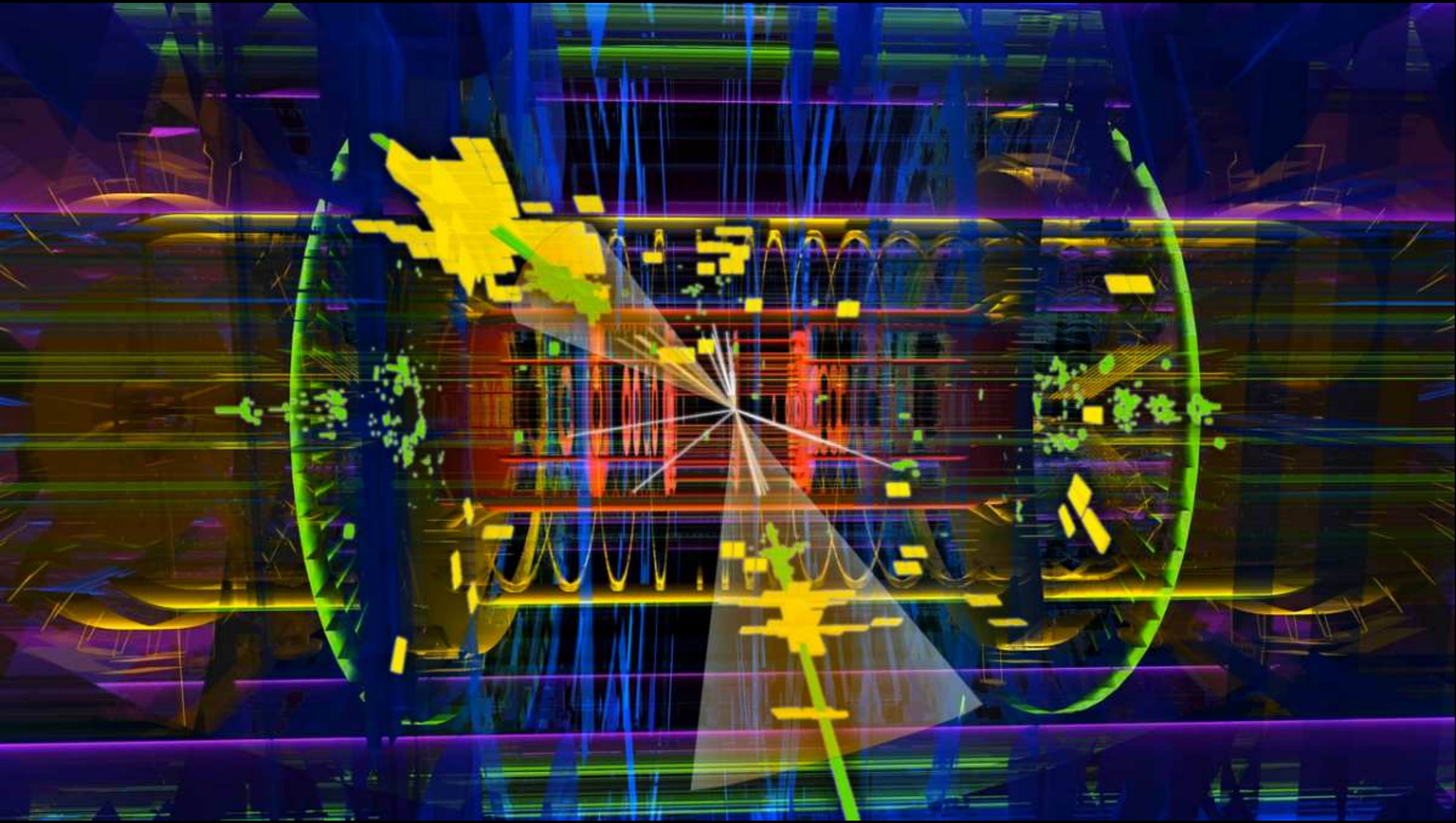
Collider Event

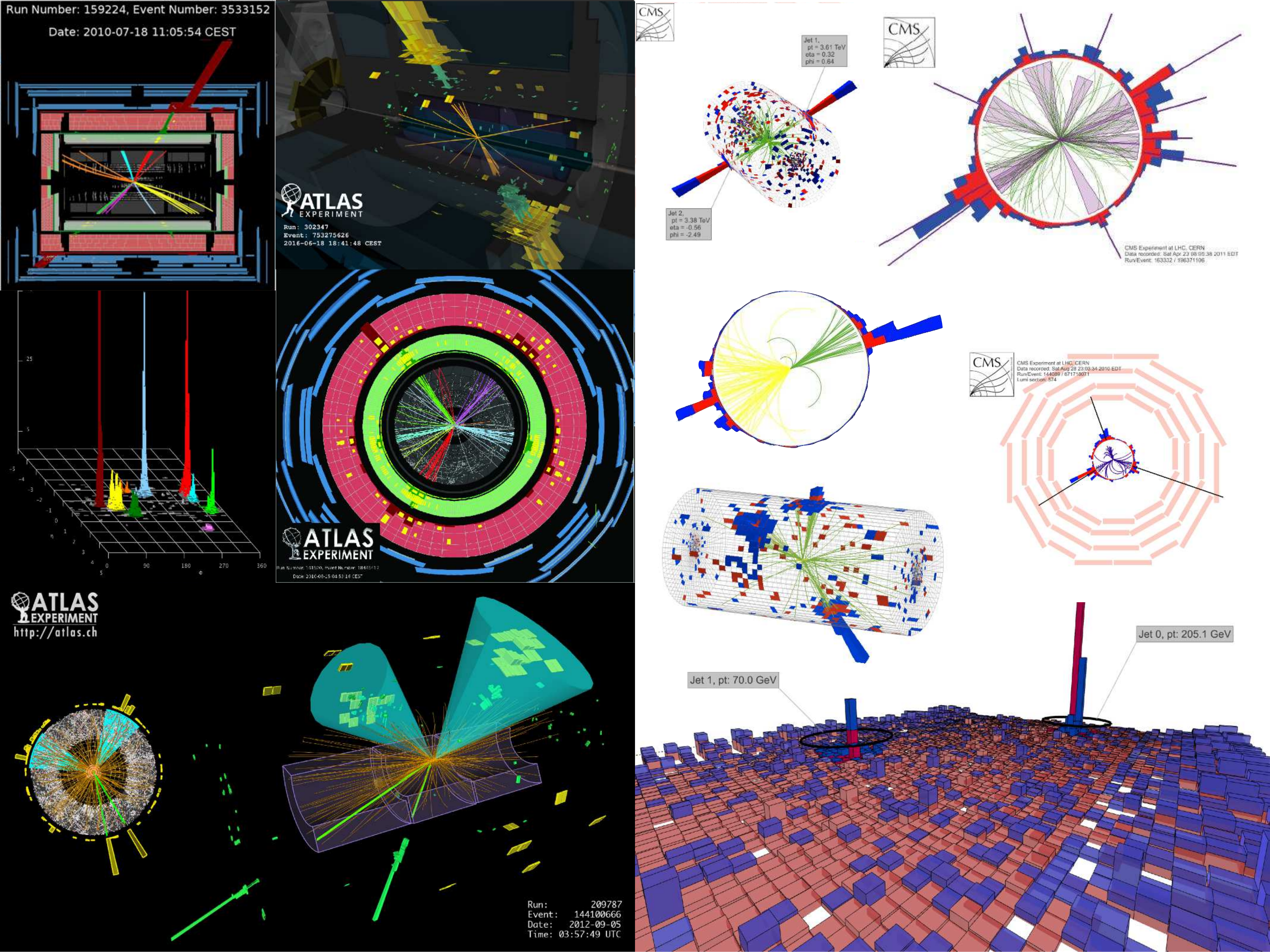
Every 25 nanoseconds at the LHC



	T	E	H	M		
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



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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
ATLAS EXPERIMENT
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

What is a "Quark Jet" vs. "Gluon Jet"?

Quark (color triplet) vs. Gluon (color octet)
But jet constituents are color-singlet hadrons!

Ill-Defined

What people sometimes think we mean

Quark as noun

Quark as adjective

Well-Defined

What we mean

A quark parton

A Born-level quark parton

The initiating quark parton in a final state shower

An eikonal line with baryon number 1/3 and carrying triplet color charge

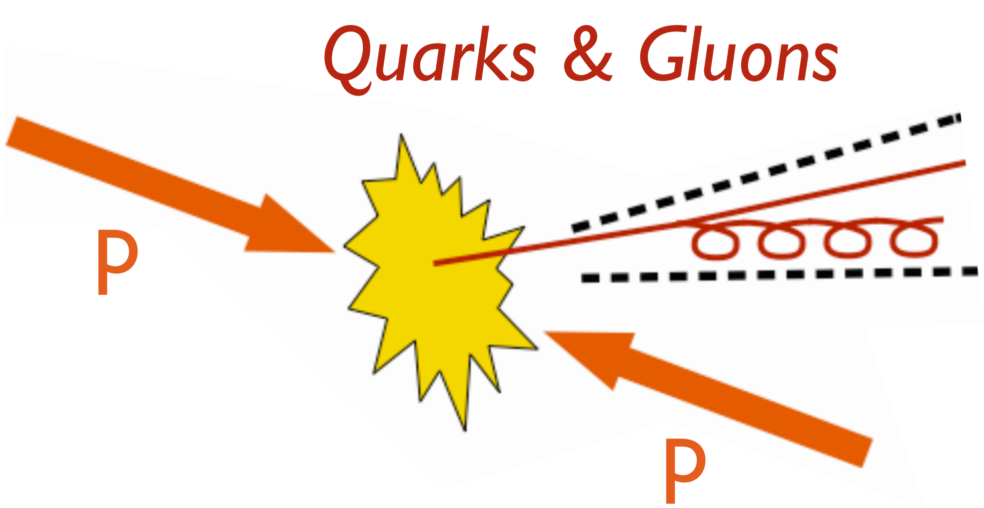
A quark operator appearing in a hard matrix element in the context of a factorization theorem

A parton-level jet object that has been quark-tagged using a soft-safe flavored jet algorithm (automatically collinear safe if you sum constituent flavors)

A phase space region (as defined by an unambiguous hadronic fiducial cross section measurement) that yields an enriched sample of quarks (as interpreted by some suitable, though fundamentally ambiguous, criterion)

[Gras, Hoeche, Kar, Larkoski, Lönnblad, Plätzer, Siódmok, Skands, Soyez, JDT, JHEP 2017; citing long history going back at least to Nilles, Streng, PRD 1981]

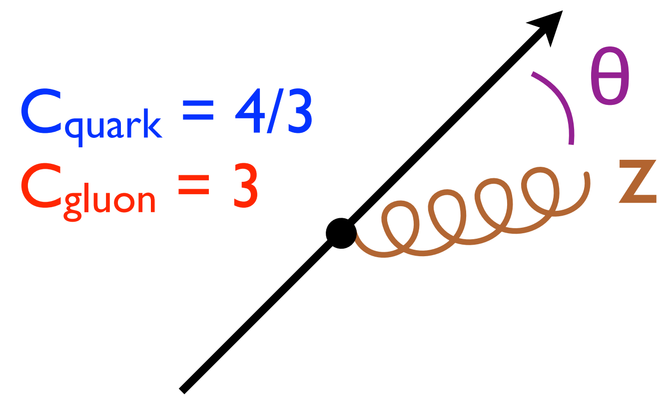
Emphasizing the Challenge



Quarks and gluons are primarily distinguished by their color charge

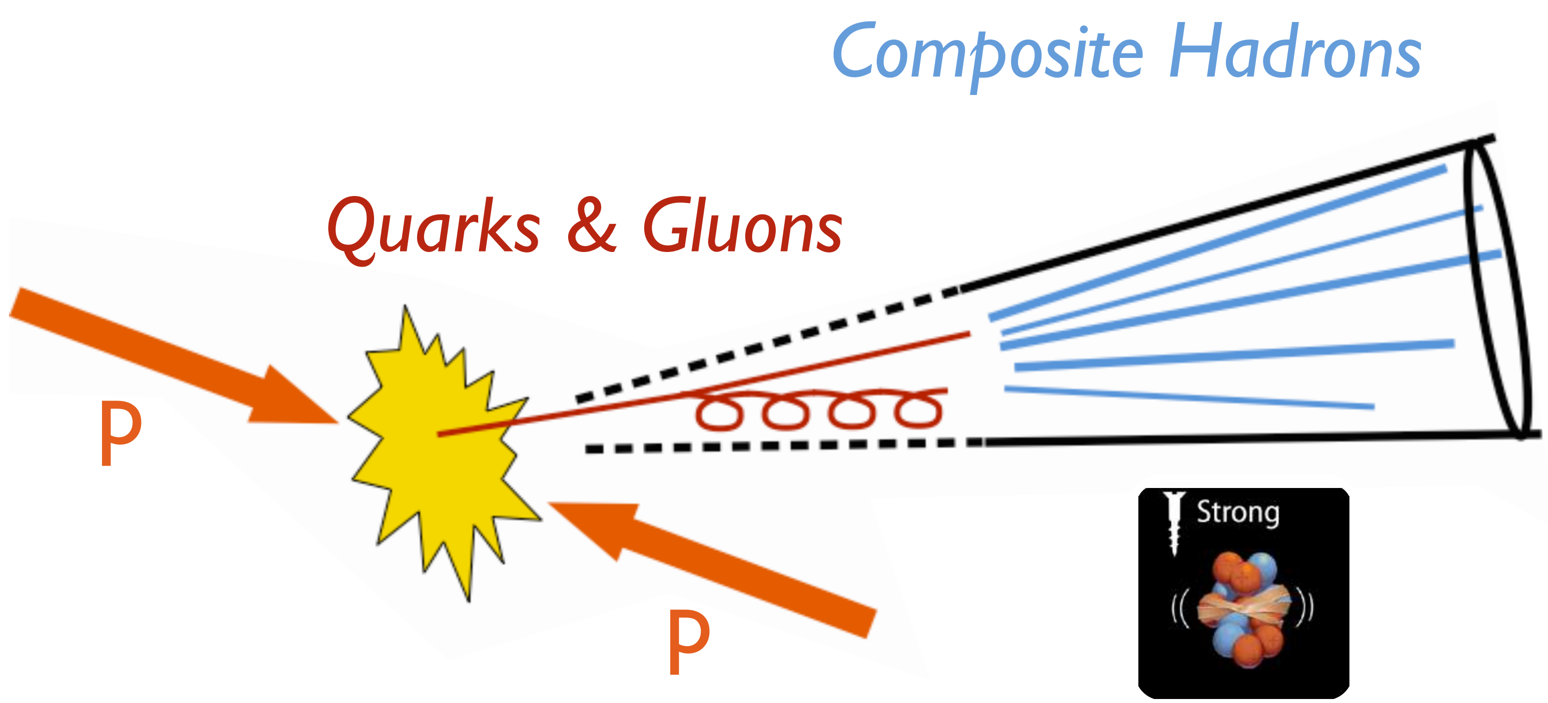
Altarelli-Parisi Splitting

Core prediction of QCD

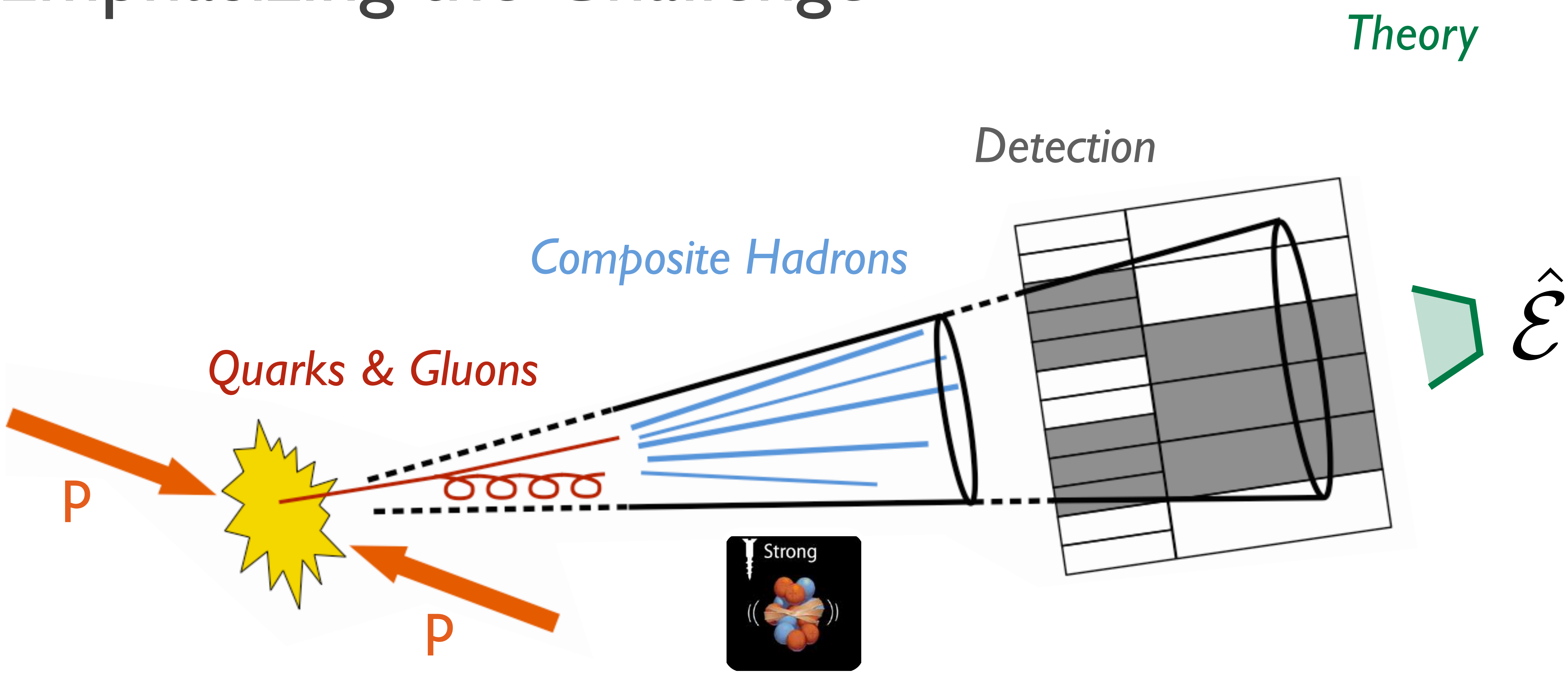


$$\mathrm{d}P_{i\to ig} \simeq \frac{2\alpha_s}{\pi} C_i \underbrace{\frac{\mathrm{d}\theta}{\theta}}_{\text{Collinear}} \underbrace{\frac{\mathrm{d}z}{z}}_{\text{Soft}}$$

Emphasizing the Challenge



Emphasizing the Challenge



Energy Flow:

Robust to hadronization and detector effects…
…but blind to direct quark/gluon information

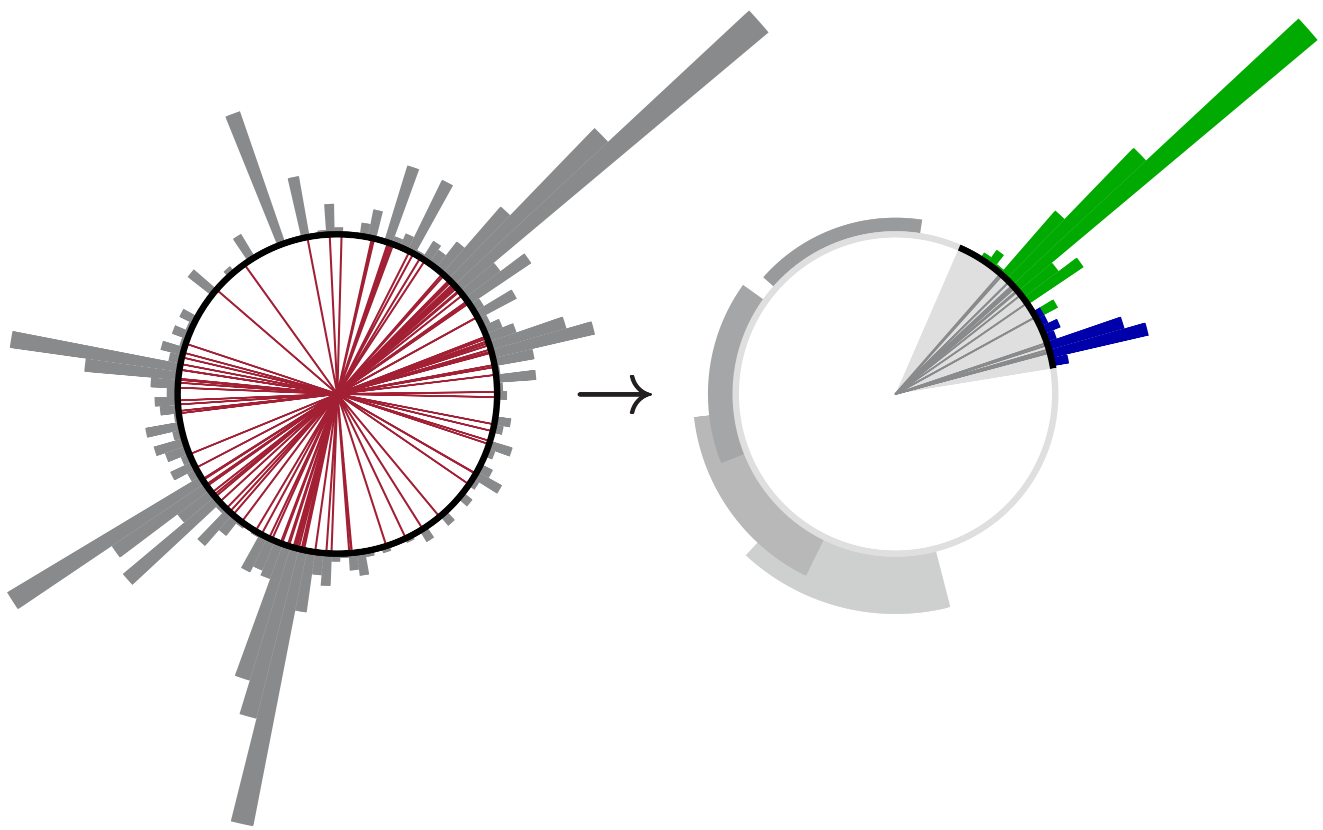
$$\boxed{\hat{\mathcal{E}} \simeq \lim_{t\to\infty} \hat{n}_i T^{0i}(t, vt\hat{n})}$$

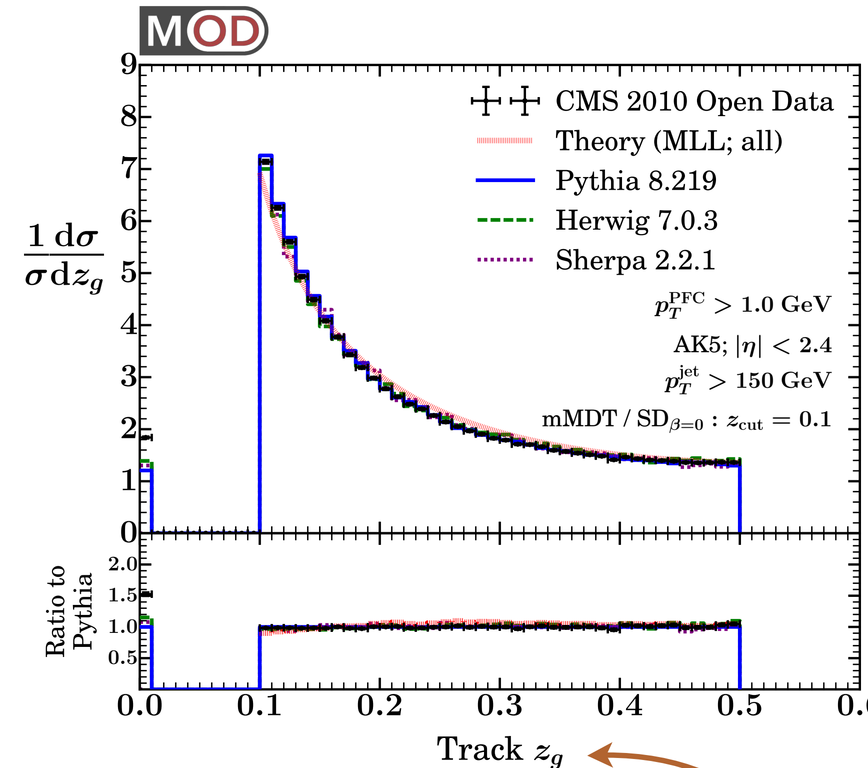
(more about this in backup)

[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]

Color-Blind Tests of QCD

First ever analysis using public LHC data!

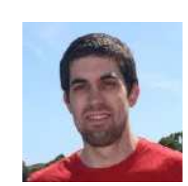


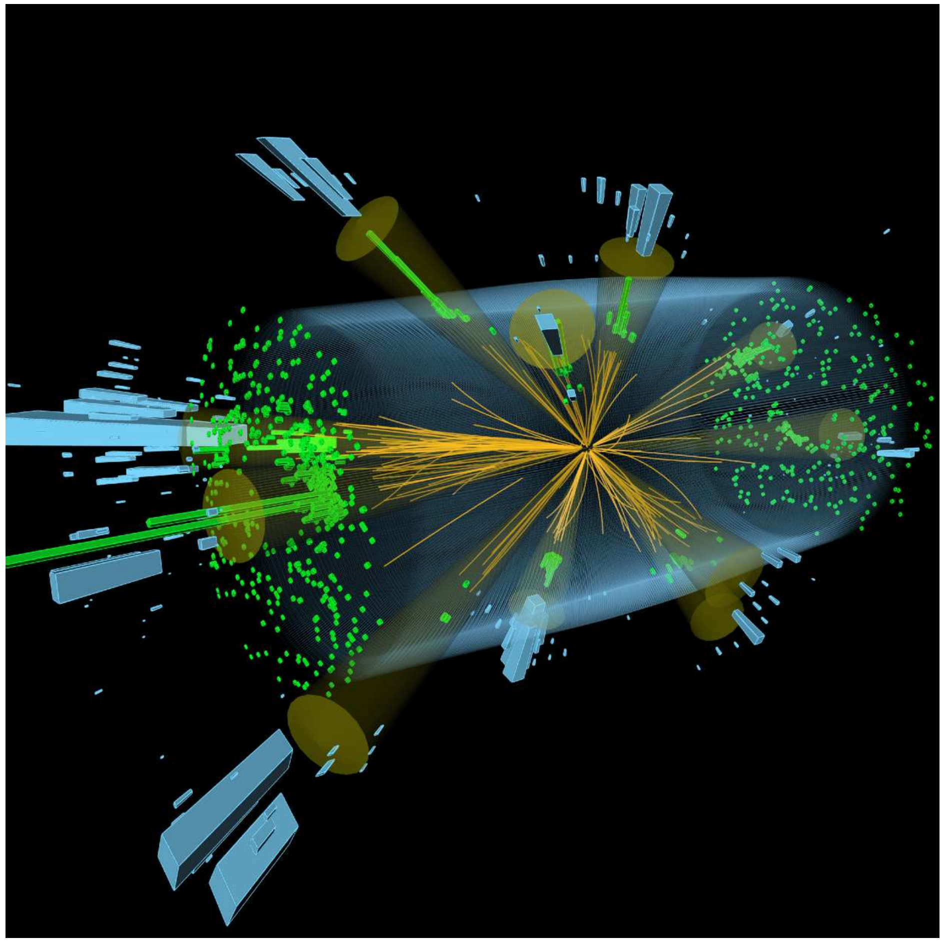


$$dP_{i\to ig} \simeq \frac{2\alpha_s}{\pi} C_i \frac{d\theta}{\theta} \frac{dz}{z}$$

Insensitive to quark/gluon composition. Can we do the opposite?!

[Tripathee, Xue, Larkoski, Marzani, JDT, PRL 2017, PRD 2017; based on Larkoski, Marzani, JDT, PRD 2015]



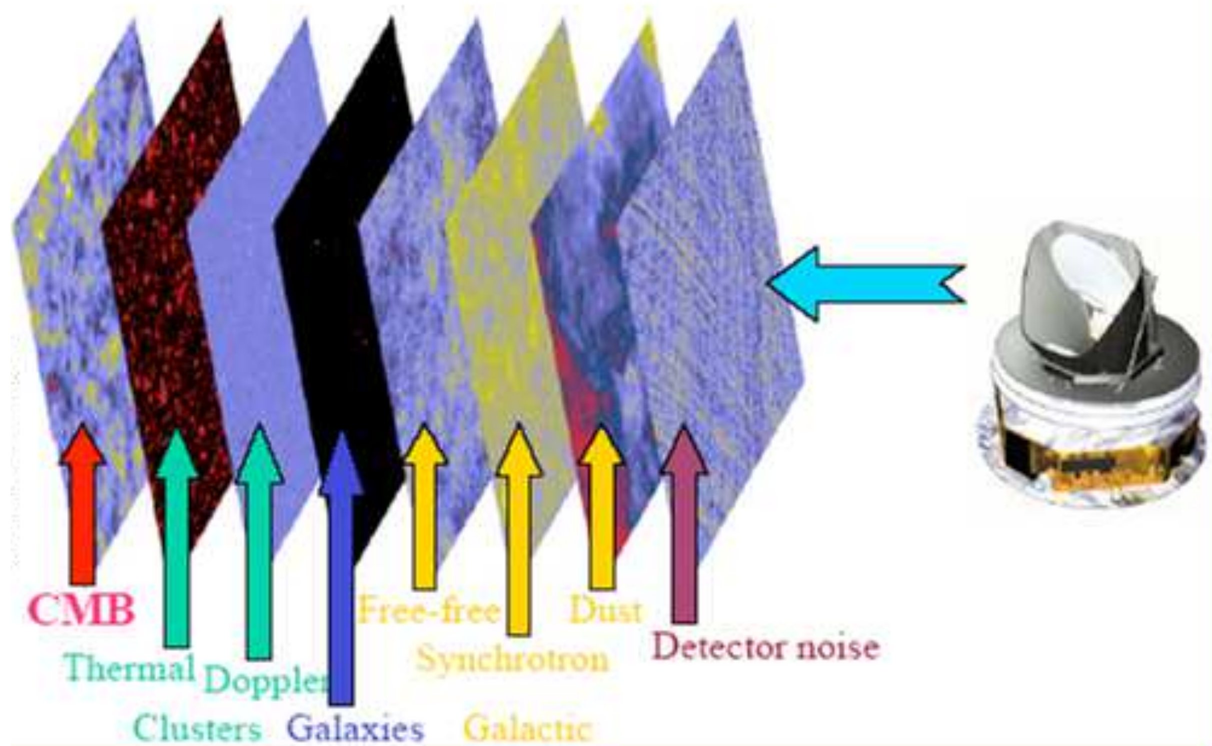
Jets are manifestation of quarks and gluons,
but there is no unambiguous way
to tell a quark jet from a gluon jet

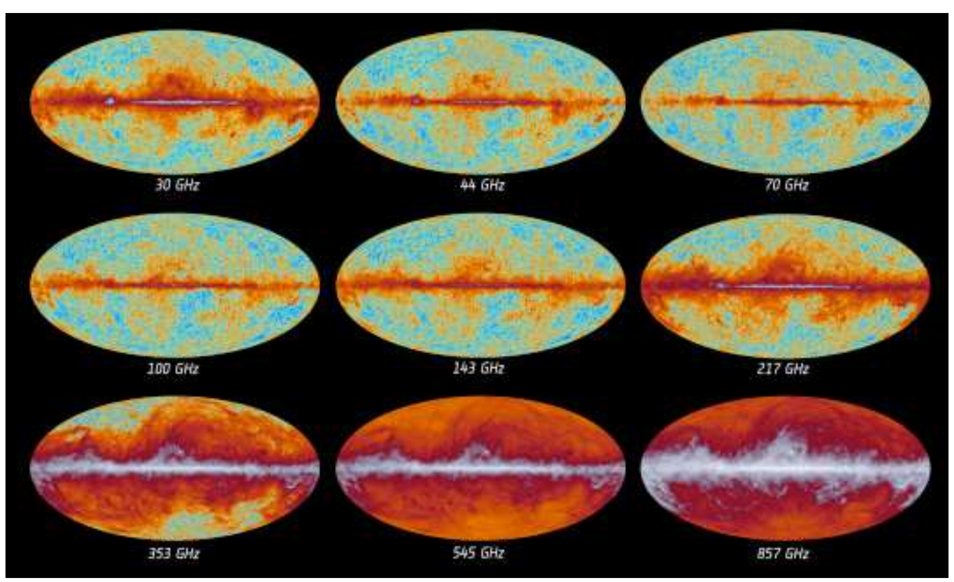
2017: A Quark/Gluon Conundrum

2018: Leveraging Weak Supervision

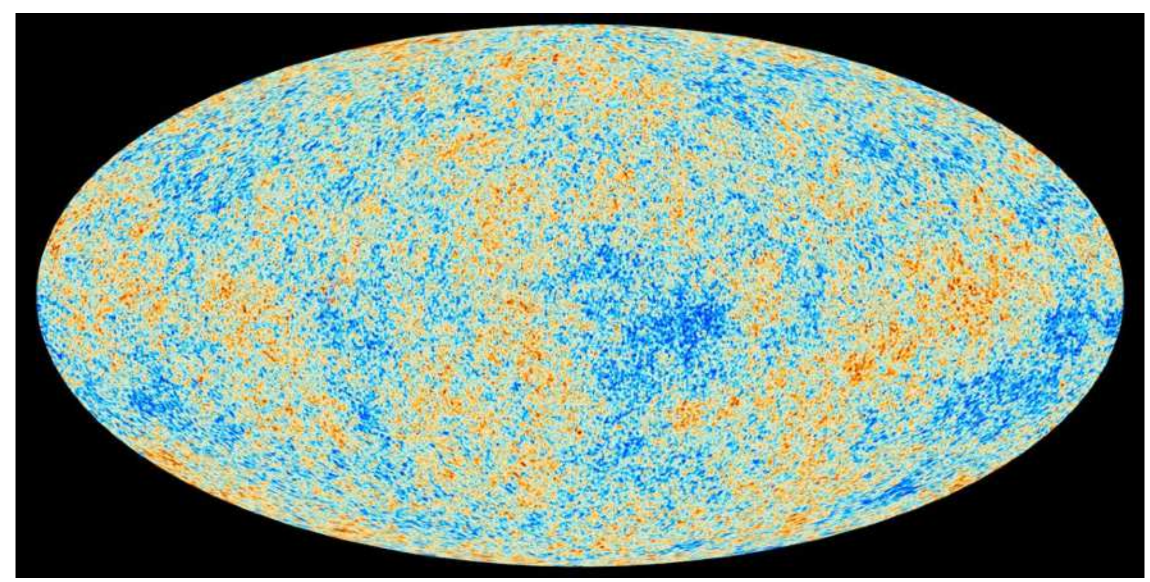
2019-2022: The Strong Force Revisited

Blind Source Separation for Cosmology





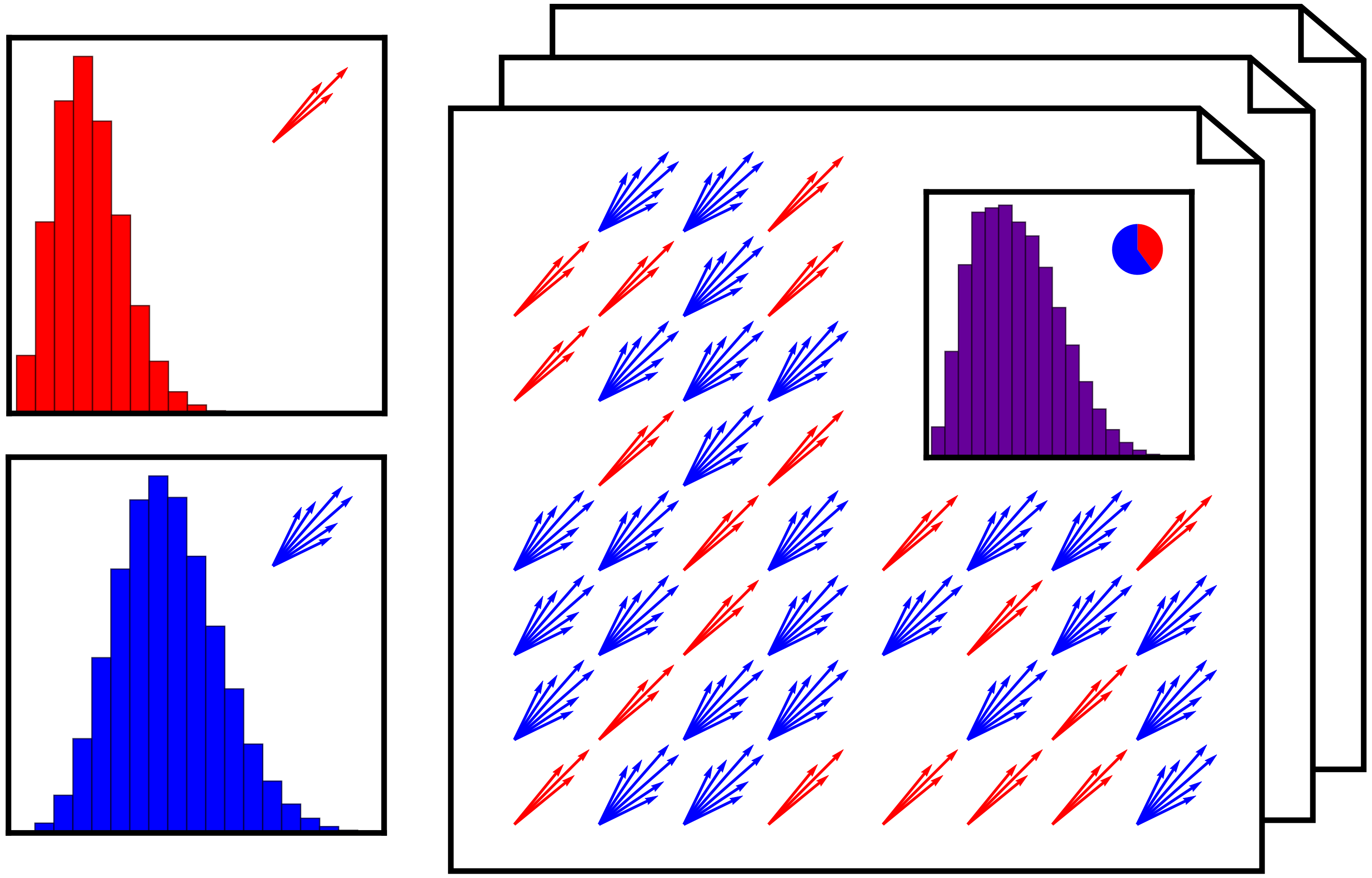
$\Rightarrow$



[Planck Outreach]

Blind Source Separation for Quark/Gluon Jets?

While you can't unambiguously label individual jets, you can extract quark and gluon distributions from hadron-level measurements



In natural language processing, this is known as "topic modeling"

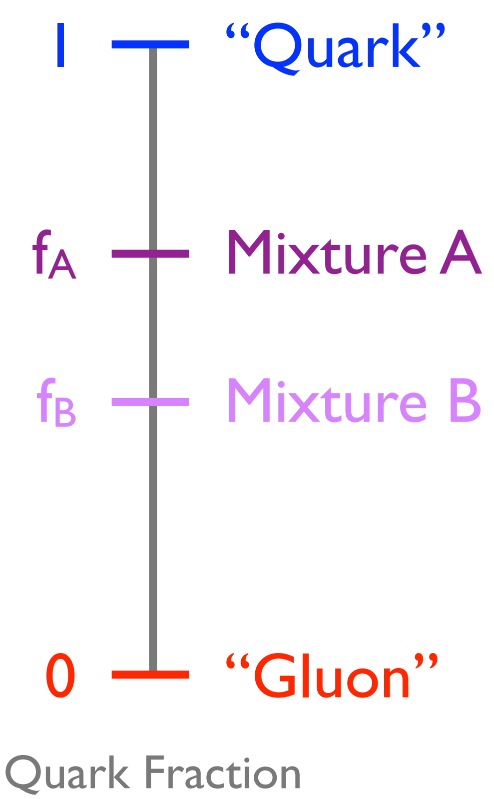
[Komiske, Metodiev, JDT, JHEP 2018; cf. ATLAS, PRD 2019; using Metodiev, Nachman, JDT, JHEP 2017; Metodiev, JDT, PRL 2018]
[see also Blanchard, Flaska, Handy, Pozzi, Scott, PLMR 2013; Katz-Samuels, Blanchard, Scott, JMLR 2016]
[Yes, for those of you obsessed with these things, I flipped the color of quark and gluon on this slide.]

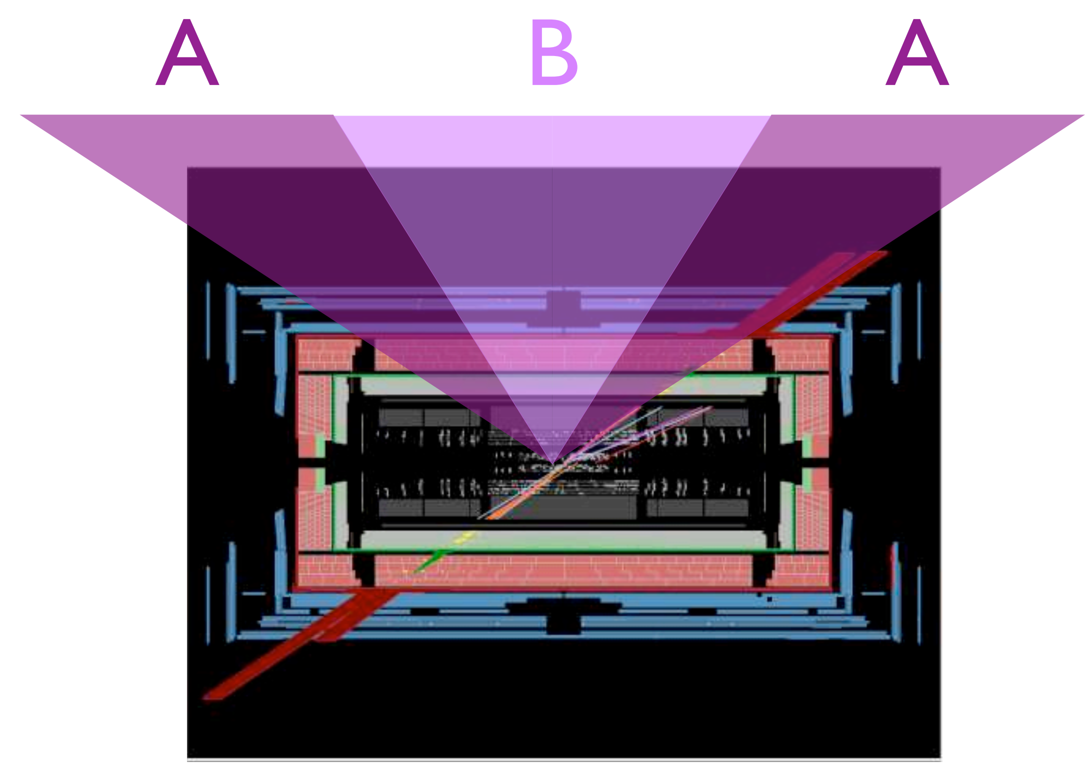
Fundamental Assumption

One can make jet samples that are mixtures of "quarks" and "gluons"

$$p_{\text{mixed}}(\vec{x}) = f_q \, p_{\text{quark}}(\vec{x}) + (1 - f_q) \, p_{\text{gluon}}(\vec{x})$$

↳ Jet Features



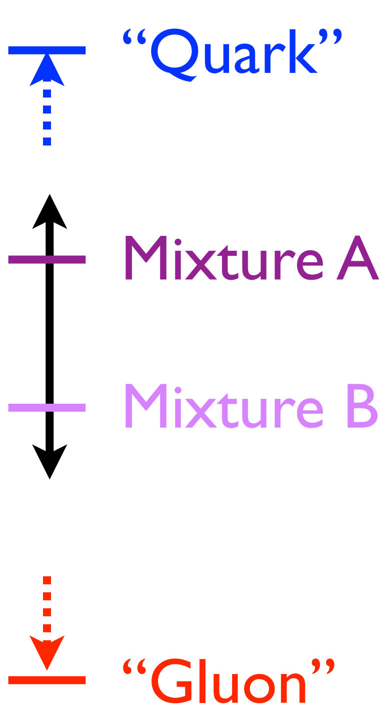


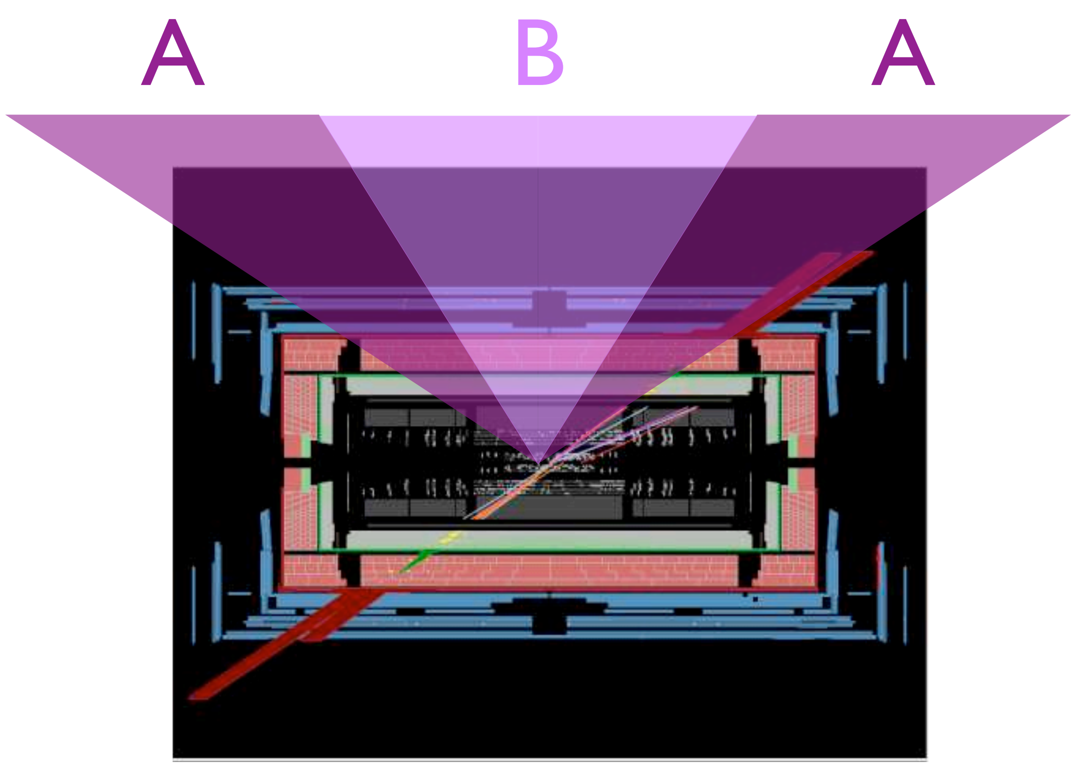
Non-trivial! Assumes A/B mixtures have unbiased jet properties

Fundamental Trick

From A/B mixtures you can *define* "quarks" and "gluons"

$$p_{\text{quark}}(\vec{x}) = \frac{p_A(\vec{x}) - \kappa_{AB}\, p_B(\vec{x})}{1 - \kappa_{AB}} \qquad p_{\text{gluon}}(\vec{x}) = \frac{p_B(\vec{x}) - \kappa_{BA}\, p_A(\vec{x})}{1 - \kappa_{BA}}$$

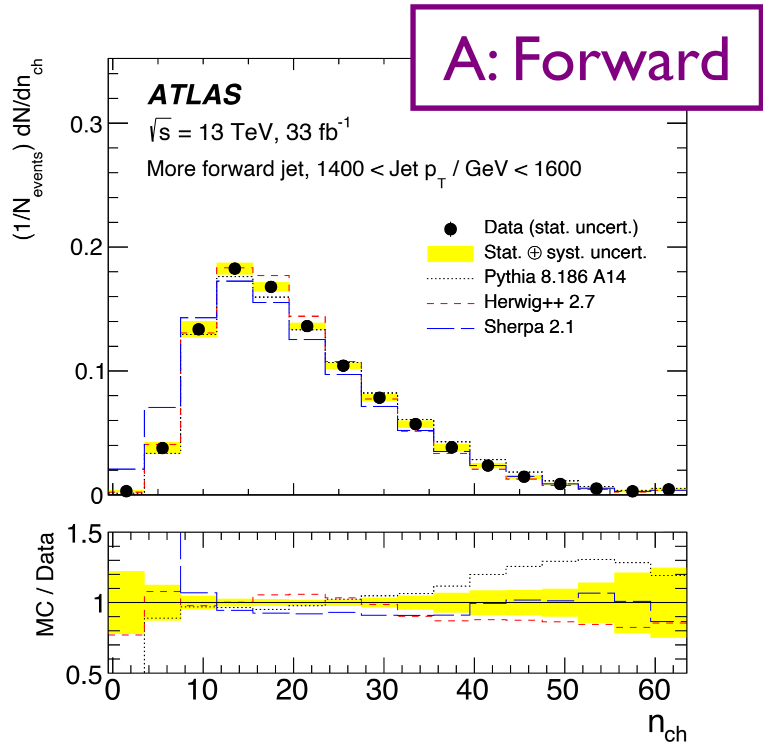


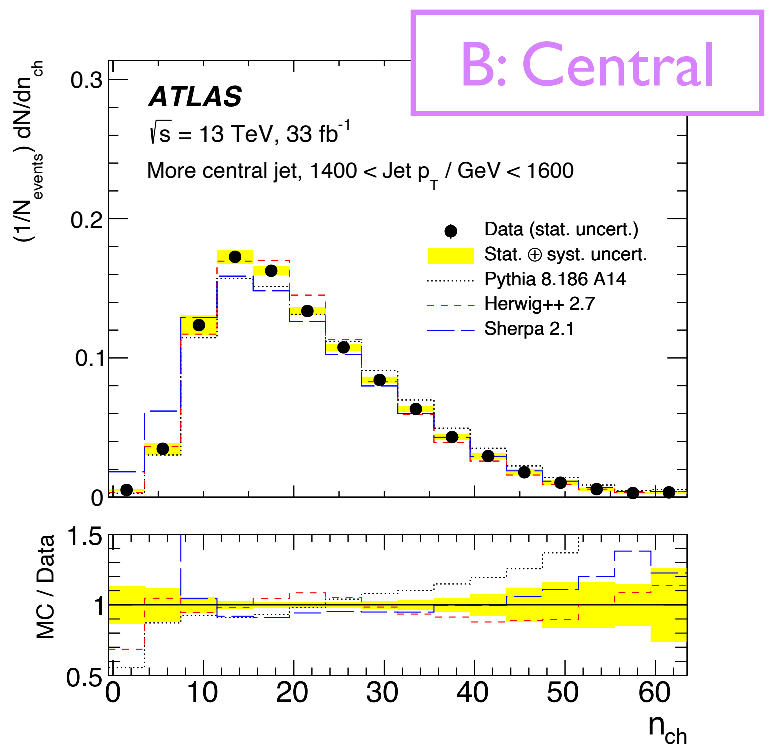


Choosing κ as big as possible yields "mutually irreducible" distributions

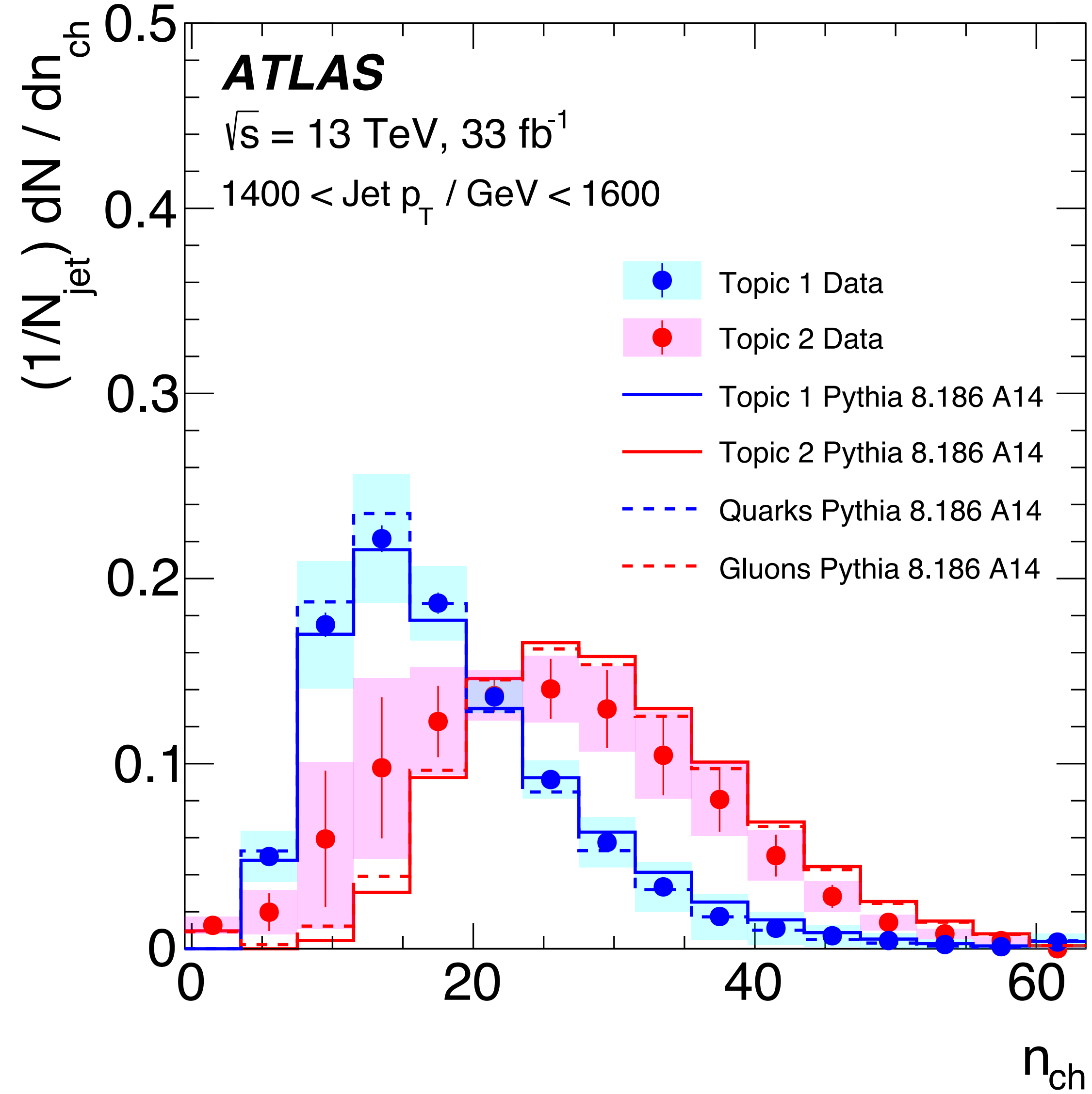
[Katz-Samuels, Blanchard, Scott, JLMR 2016; advocated for in Komiske, Metodiev, JDT, JHEP 2018]

Jet Topics Result from ATLAS





Track multiplicity for "Topic 1" and "Topic 2"



[ATLAS, PRD 2019]

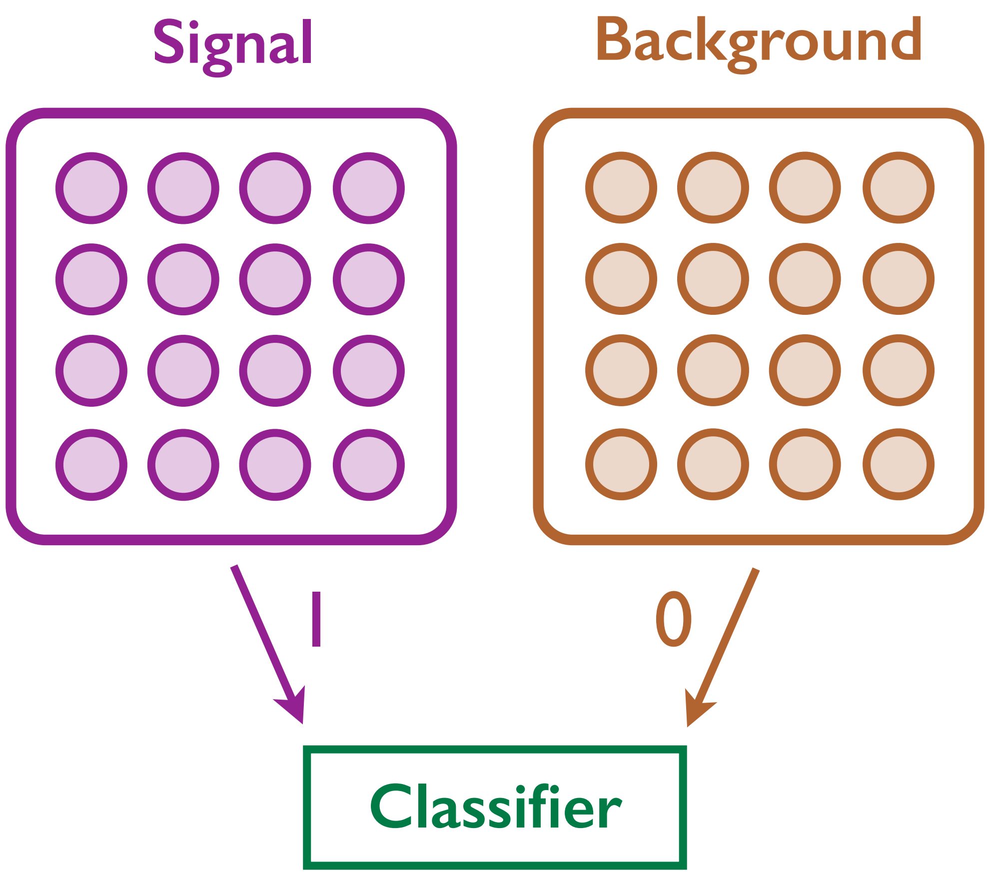
"Ok, but don't jet topics depend on choice of jet features?"

Yes! But to find maximal separability,
we can leverage weak supervision!
CWoLa = Classification Without Labels

(More accurately, classification with noisy labels)

Strong: Fully-Supervised Binary Classification

Training on pure, perfectly labeled examples



Minimize Loss Function

(asymptotically)

$$h(\vec{x}) = \frac{p_{\text{sig}}(\vec{x})}{p_{\text{sig}}(\vec{x}) + p_{\text{bkgd}}(\vec{x})}$$

Optimal Classifier (Neyman–Pearson)

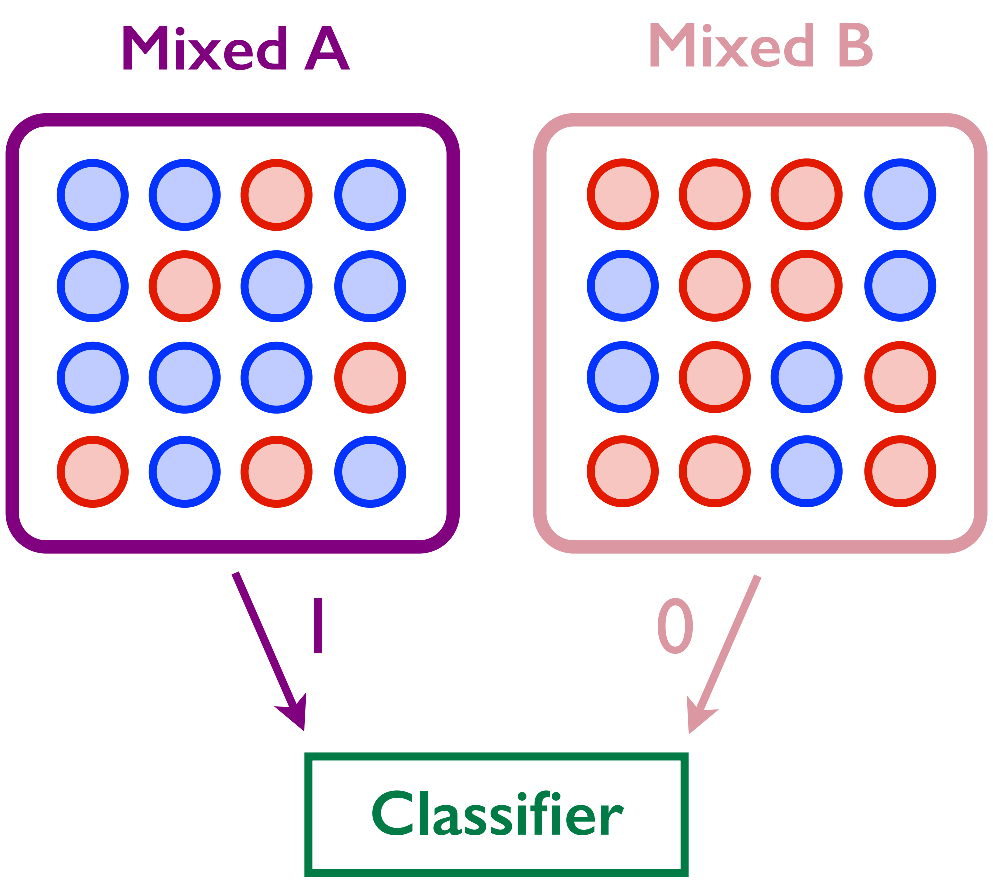
$$\ell_{\text{MSE}} = \Big\langle \big(h(\vec{x}) - 1\big)^2 \Big\rangle_{\text{signal}} + \Big\langle \big(h(\vec{x}) - 0\big)^2 \Big\rangle_{\text{background}}$$

Classifier Inputs

(See backup for Lagrangian formulation of what this is doing)

Weak: Classification Without Labels (CWoLa)

Train directly on mixed data!



$$h_{\mathrm{mixed}}(\vec{x}) = \frac{p_A(\vec{x})}{p_A(\vec{x}) + p_B(\vec{x})}$$

$$\neq$$

$$h_{\mathrm{pure}}(\vec{x}) = \frac{p_q(\vec{x})}{p_q(\vec{x}) + p_g(\vec{x})}$$

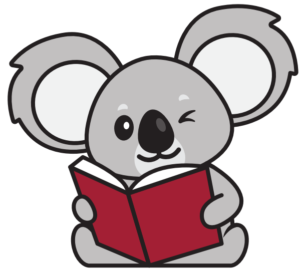
but… $$\frac{\partial h_{\mathrm{mixed}}(\vec{x})}{\partial h_{\mathrm{pure}}(\vec{x})} > 0$$

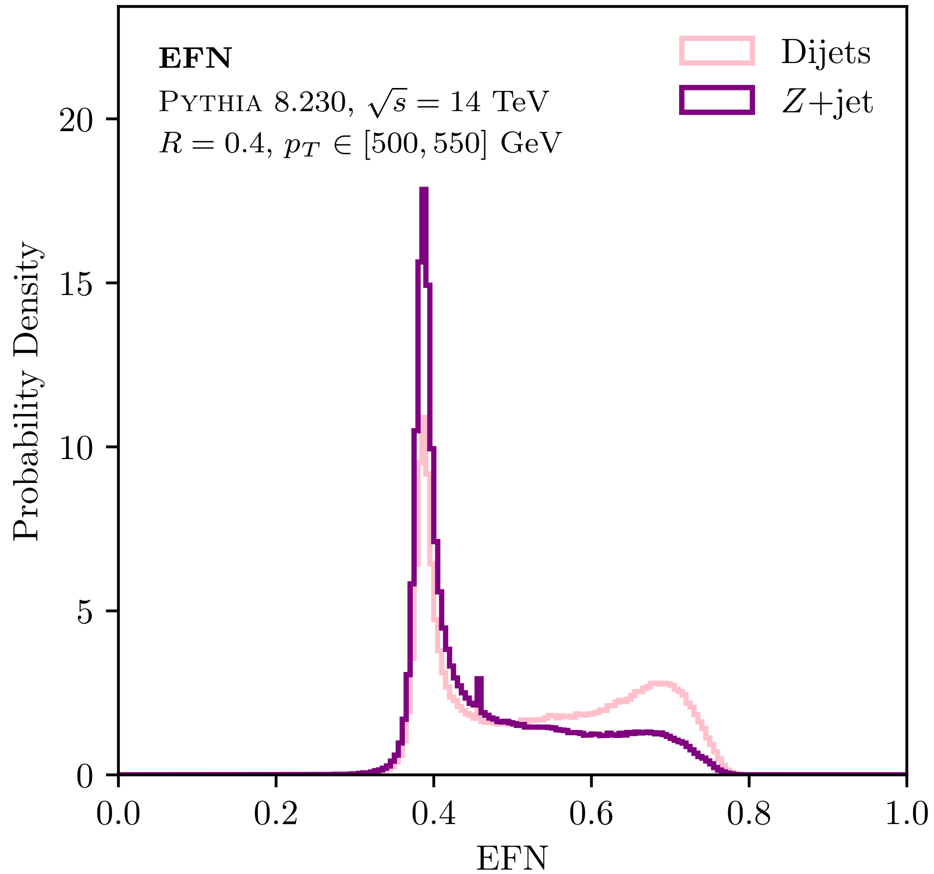
Weak supervision yields same decision boundaries as strong supervision!

[Metodiev, Nachman, JDT, JHEP 2017; see also Blanchard, Flaska, Handy, Pozzi, Scott, PLMR 2013; Cranmer, Pavez, Louppe, arXiv 2015; Dery, Nachman, Rubbo, Schwartzman, JHEP 2017; Cohen, Freytsis, Ostdiek, JHEP 2018; Komiske, Metodiev, Nachman, Schwartz, PRD 2018; Collins, Howe, Nachman, PRL 2018, PRD 2019]

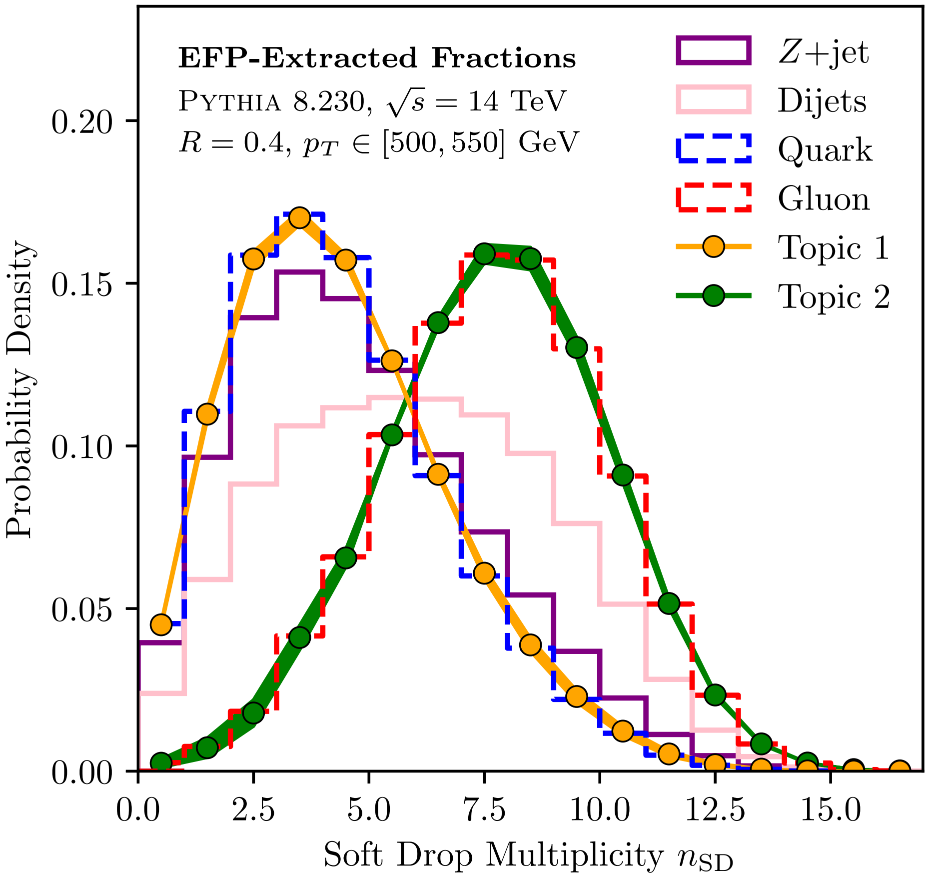
The Well-Read CWoLa

Weak supervision meets topic modeling





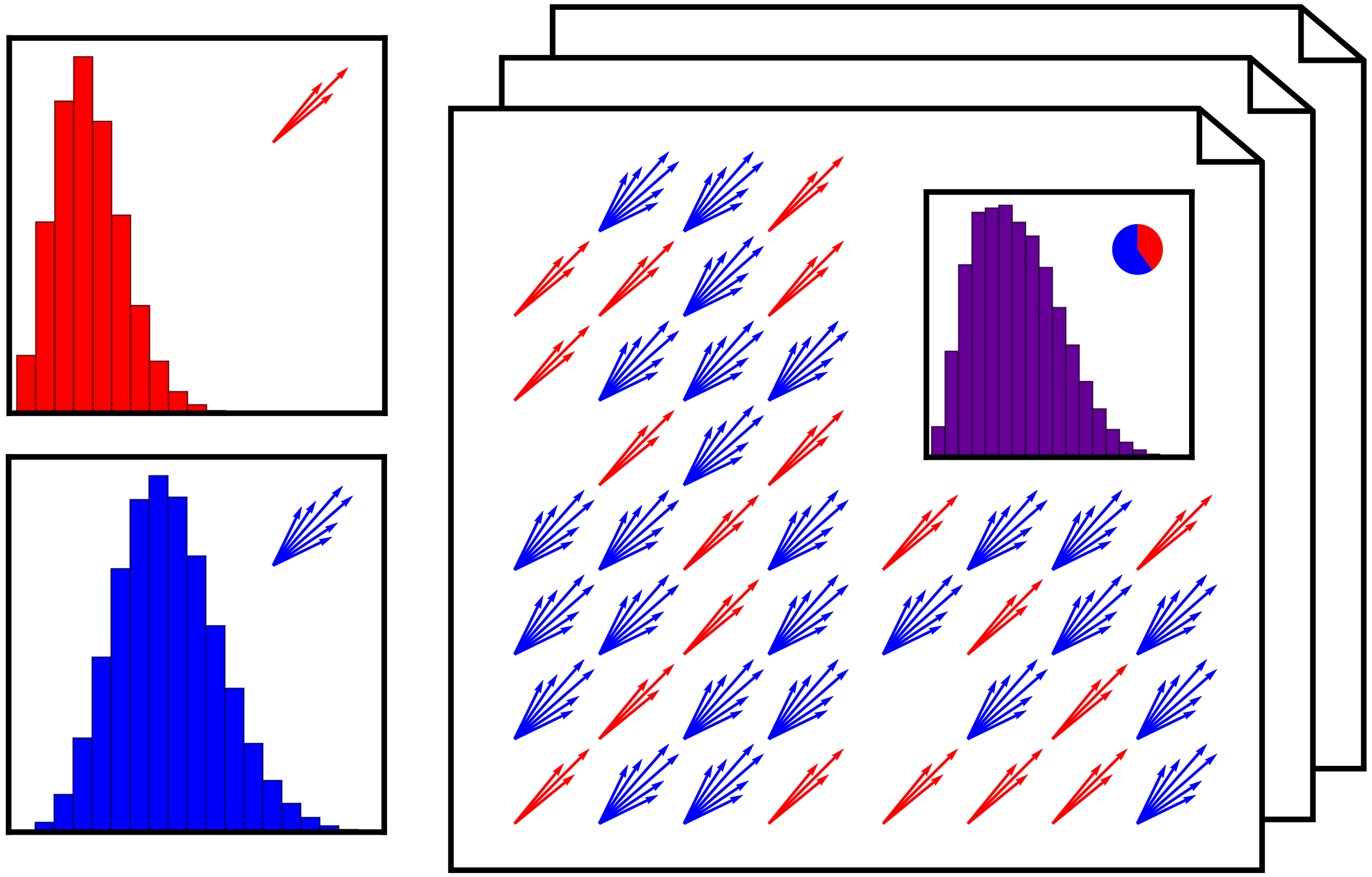
$\Rightarrow$



$$h_{\text{pure}} \in [0, 1]$$

$$h_{\text{mixed}} \in \left[\frac{f_g^A}{f_g^A + f_g^B}, \frac{f_q^A}{f_q^A + f_q^B}\right]$$

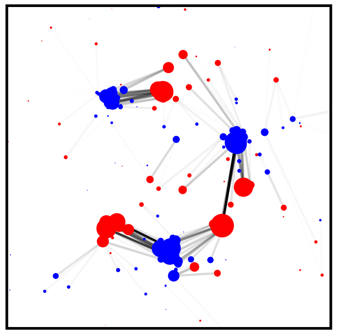
[Komiske, Metodiev, JDT, JHEP 2018]
[using Katz-Samuels, Blanchard, Scott, JLMR 2016; Metodiev, Nachman, JDT, JHEP 2017; Metodiev, JDT, PRL 2018]



By assuming jet samples are mixtures of "quarks" and "gluons", one can operationally define jet categories

2017: A Quark/Gluon Conundrum

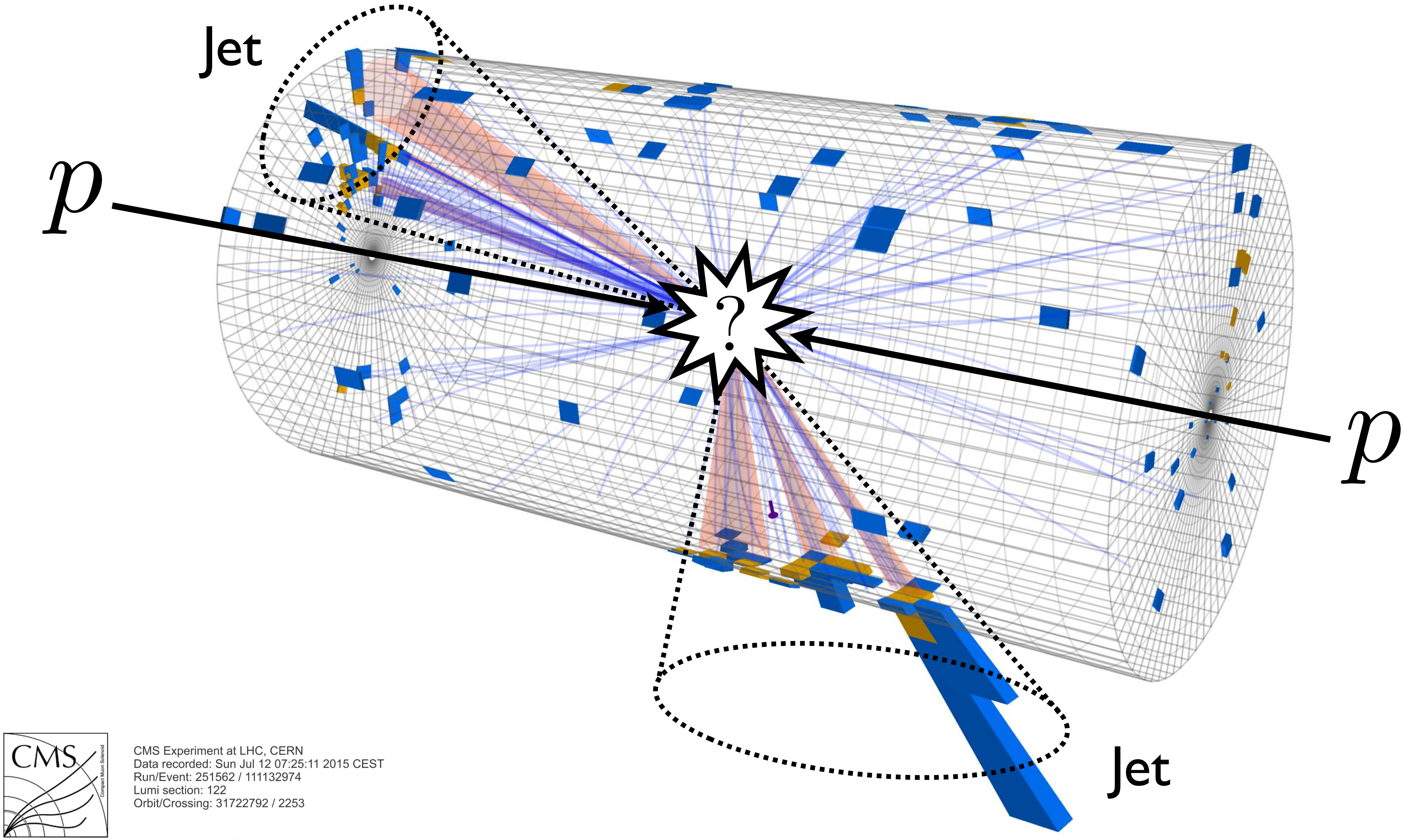
2018: Leveraging Weak Supervision



2019-2022: The Strong Force Revisited

“Collision Course”

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



“Collision Course”

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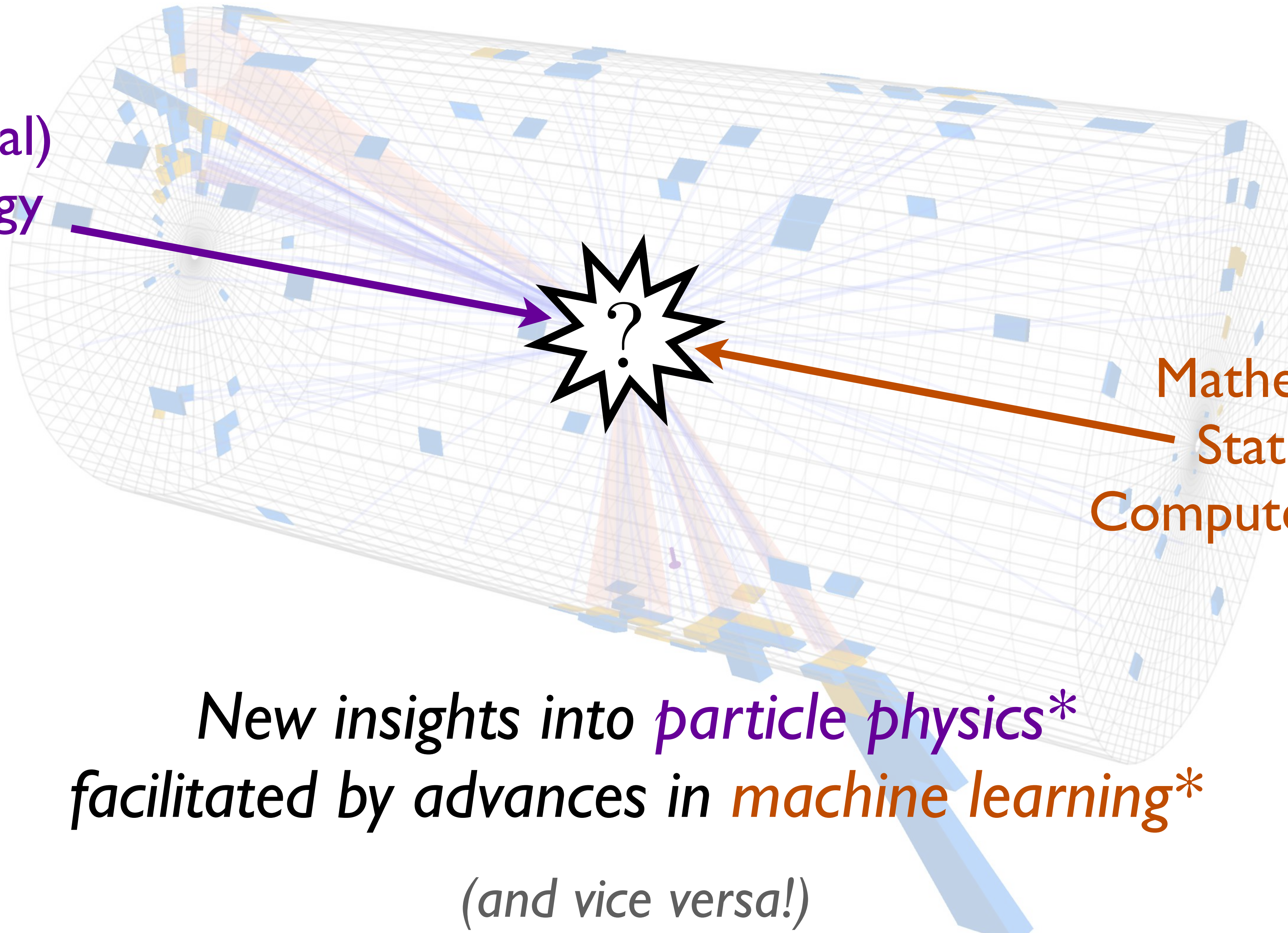


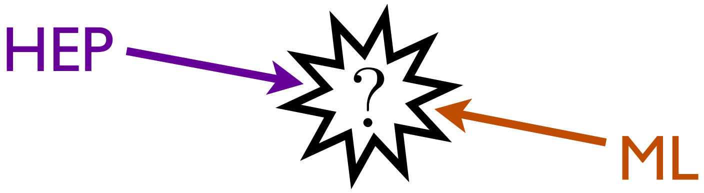
*New insights into particle physics**
*facilitated by advances in machine learning**

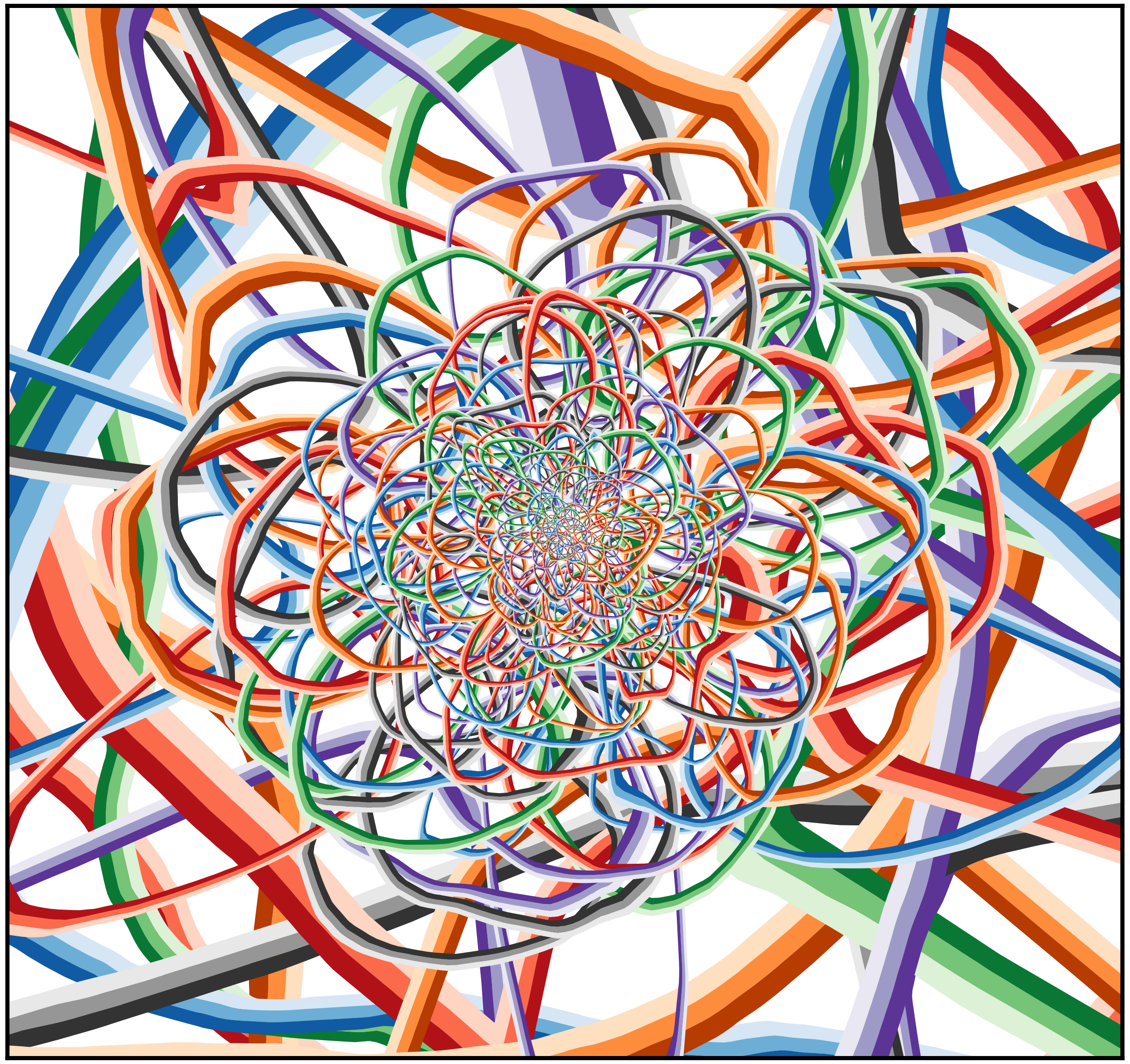
(and vice versa!)

Cue the Montage!

2019: Point Cloud Learning

Energy Flow Networks





Set-based architecture with interpretable latent space:

$$S(\mathcal{J}) = F\big(V_1, V_2, \ldots, V_\ell\big)$$

$$V_a(\mathcal{J}) = \sum_{i \in \mathcal{J}} E_i \, \Phi_a(\hat{n}_i)$$

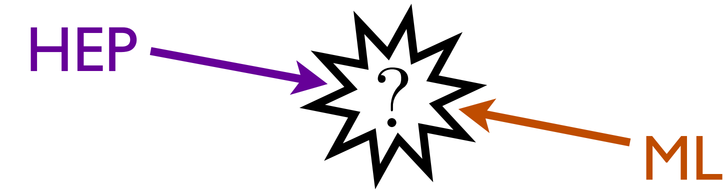
Collinear singularity of QCD!

$$\mathrm{d}P_{i \to ig} \simeq \frac{2\alpha_s}{\pi} C_i \frac{\mathrm{d}\theta}{\theta} \frac{\mathrm{d}z}{z}$$

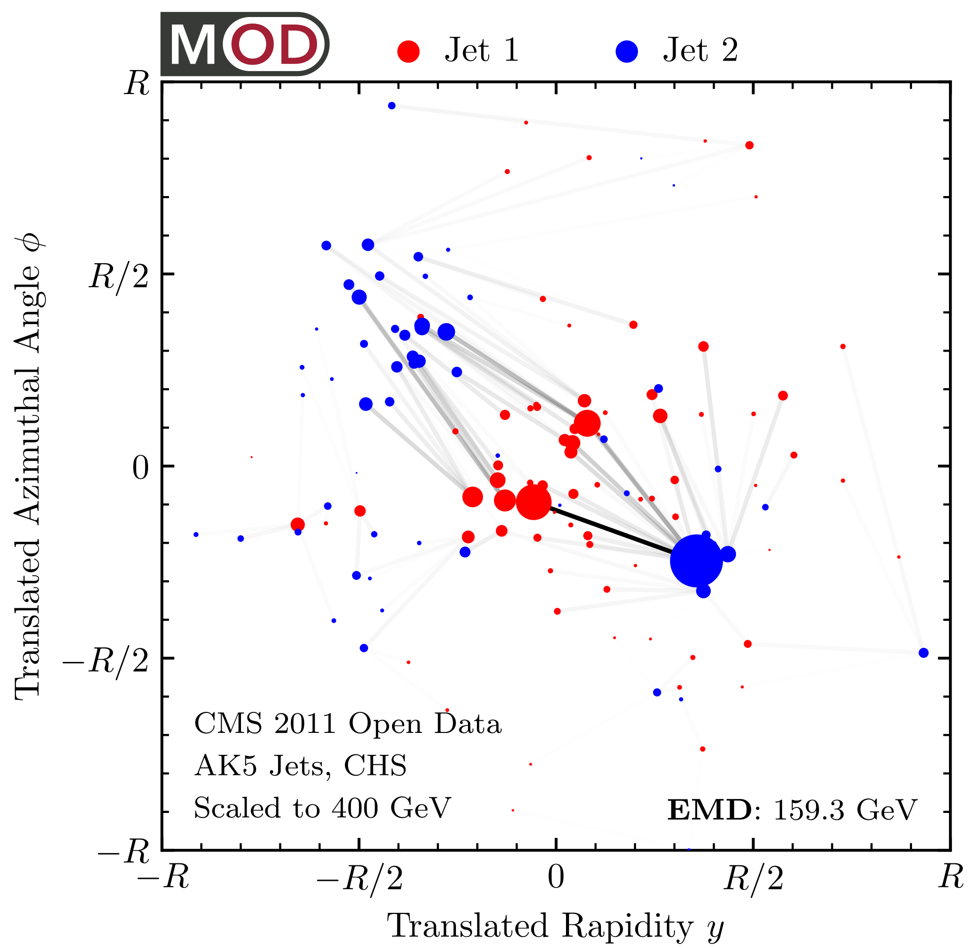
[Komiske, Metodiev, JDT, JHEP 2019; see also Komiske, Metodiev, JDT, JHEP 2018; code at energyflow.network; special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, NIPS 2017; other set-based architecture in Qu, Gouskos, PRD 2020; Mikuni, Canelli, EPJP 2020; Dolan, Ore, arXiv 2020]

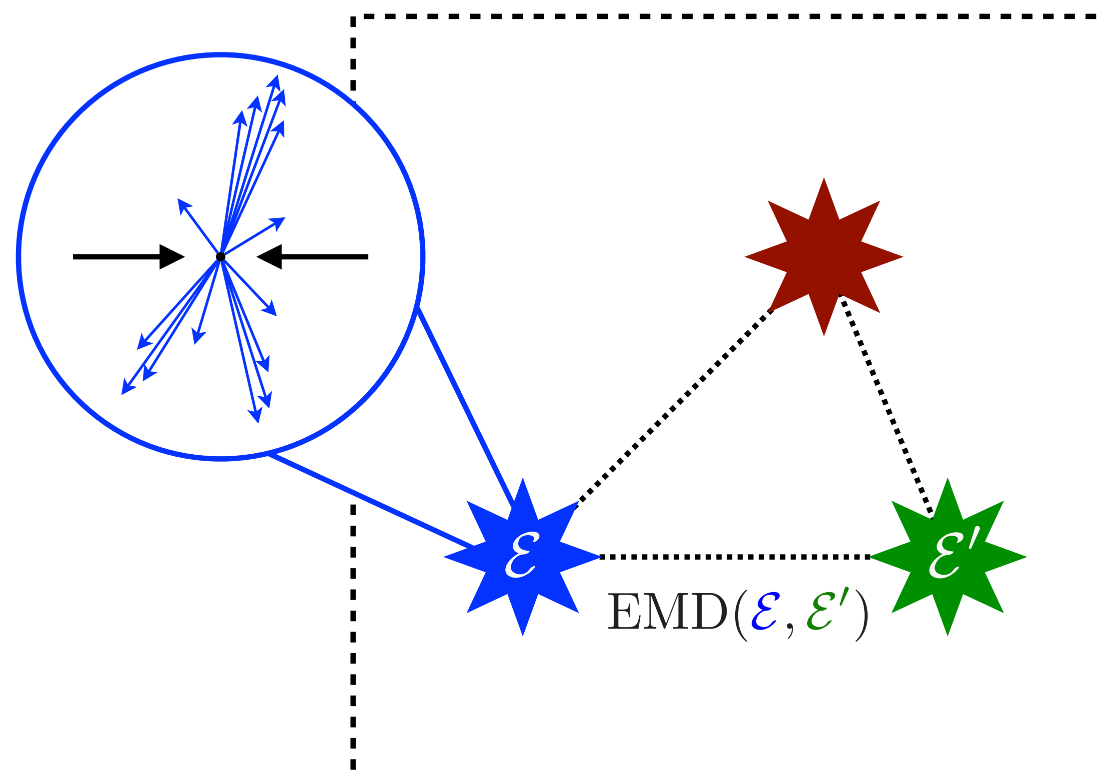
2019: Metric Space for Colliders

Energy Mover's Distance



Optimal Transport for Collider Geometry

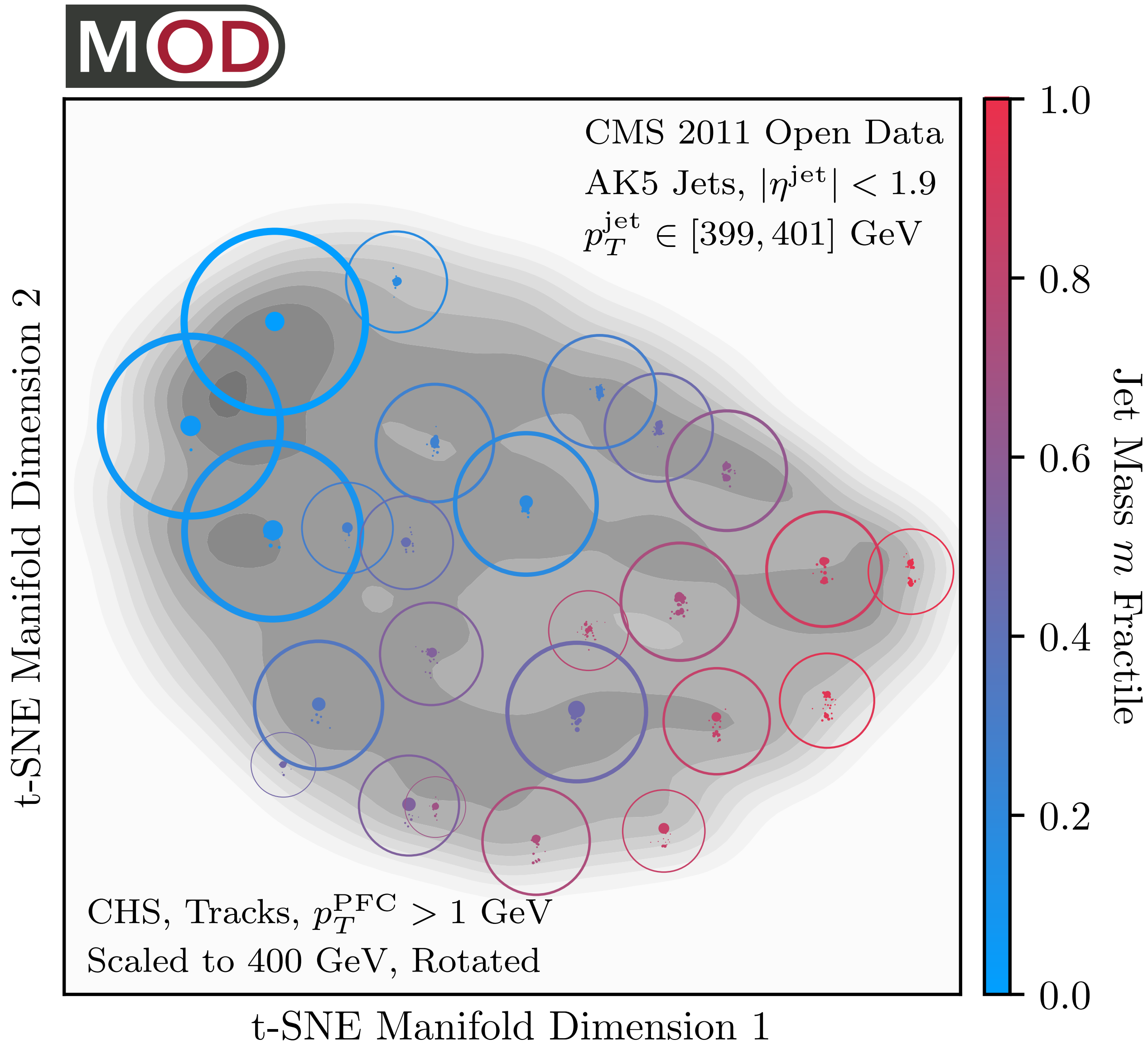




[Komiske, Metodiev, JDT, PRL 2019; code at Komiske, Metodiev, JDT, energyflow.network; open data study in Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020]
[based on Peleg, Werman, Rom, IEEE 1989; Rubner, Tomasi, Guibas, ICCV 1998, ICJV 2000; Pele, Werman, ECCV 2008; Pele Taskar, GSI 2013]
[flavored variant in Crispim Romão, Castro, Milhano, Pedro, Vale, EPJC 2021; linearized and unbalanced transport in Cai, Cheng, Craig, Craig, PRD 2020, PRD 2022]

2020: Metric Space in Open Data

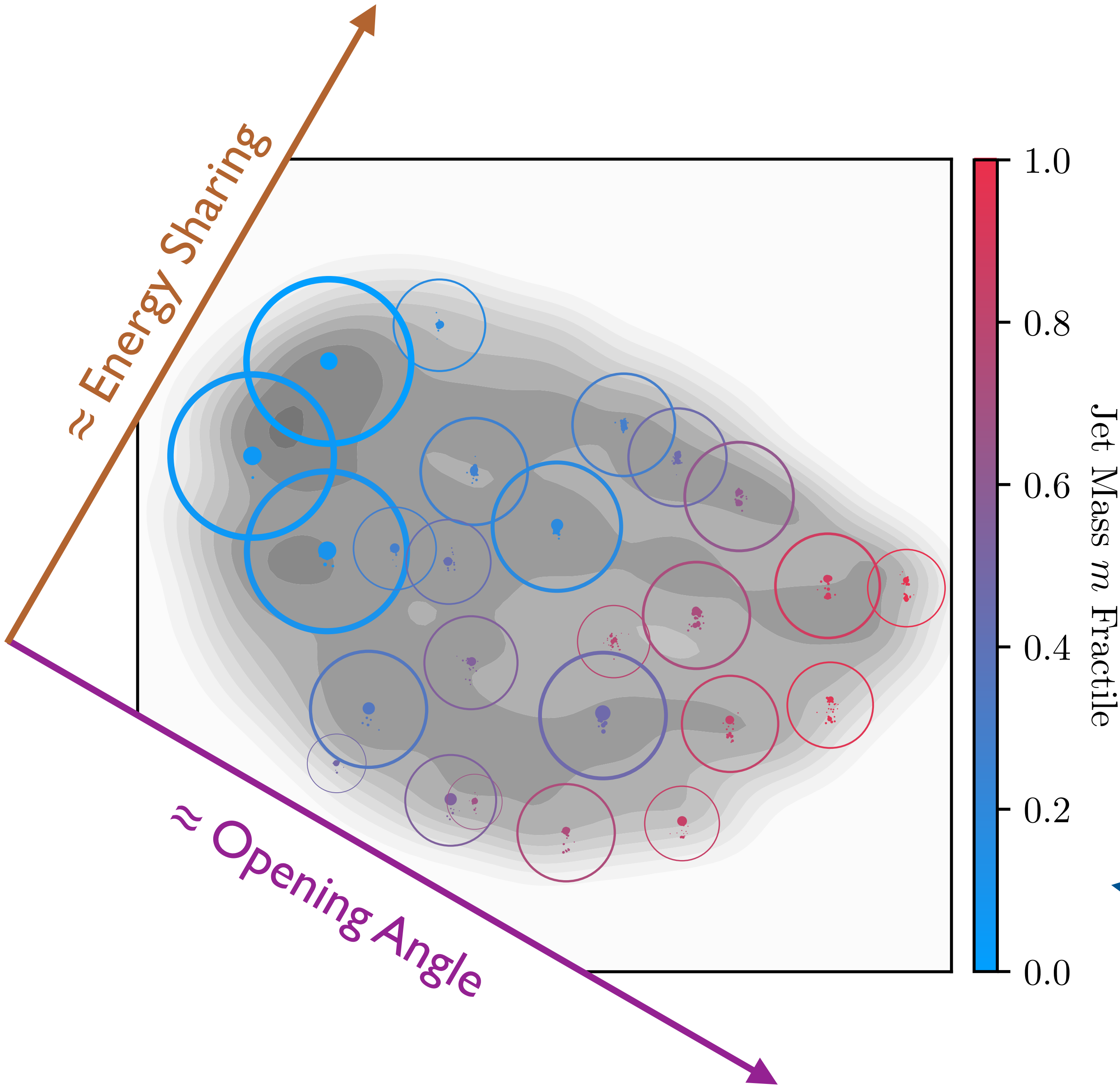
t-SNE Projection



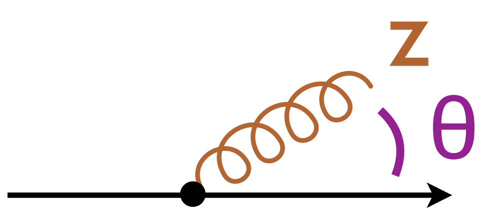
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;
using van der Maaten, Hinton, JMLR 2008; using CMS Open Data]

2020: Metric Space in Open Data

t-SNE Projection



Coordinate system of QCD!

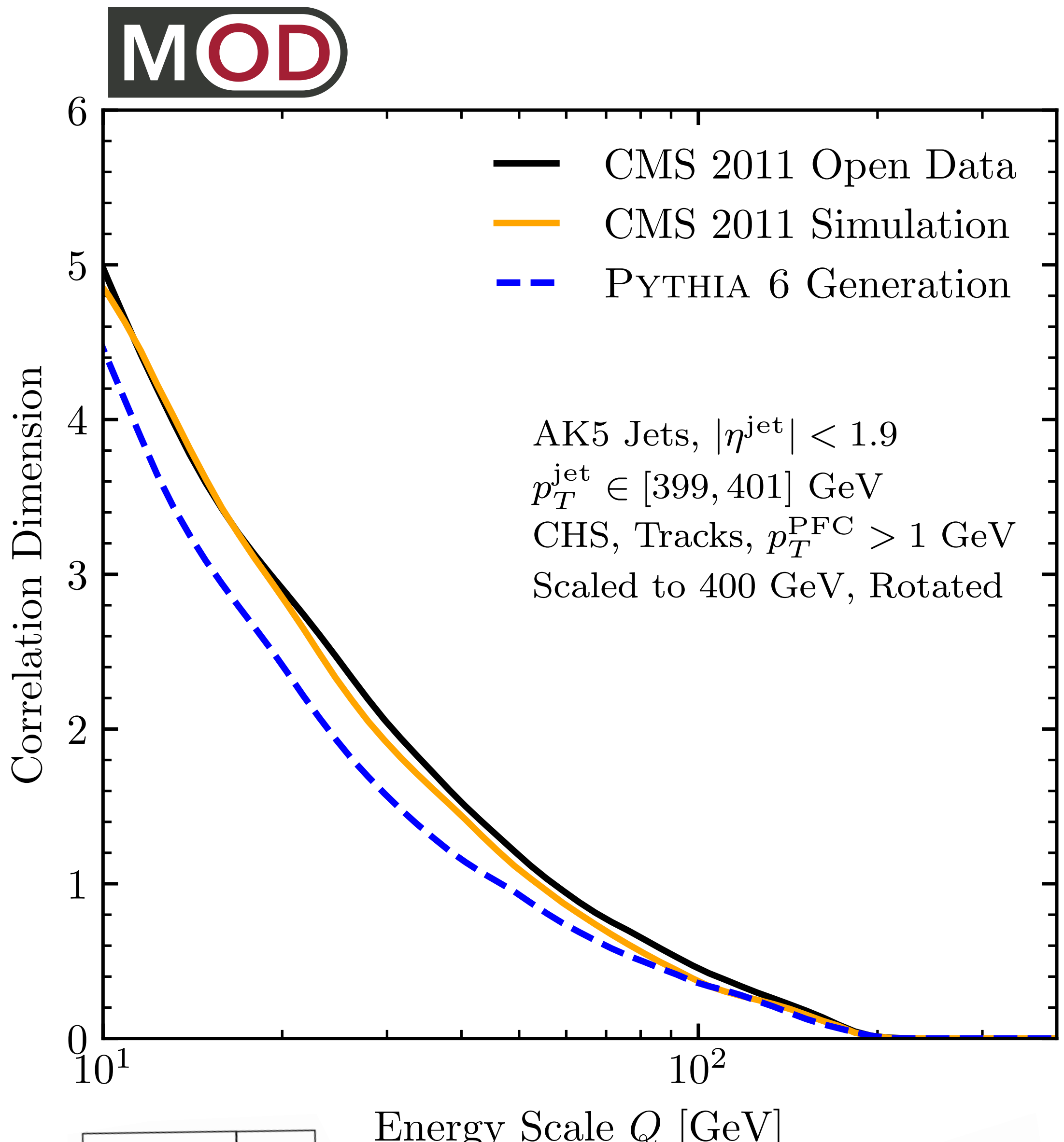


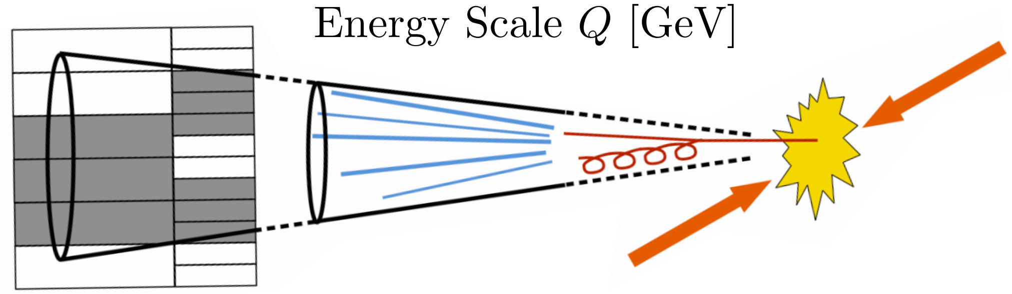
$$dP_{i\to ig} \simeq \frac{2\alpha_s}{\pi} C_i \frac{d\theta}{\theta} \frac{dz}{z}$$

[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;
using van der Maaten, Hinton, JMLR 2008; using CMS Open Data]

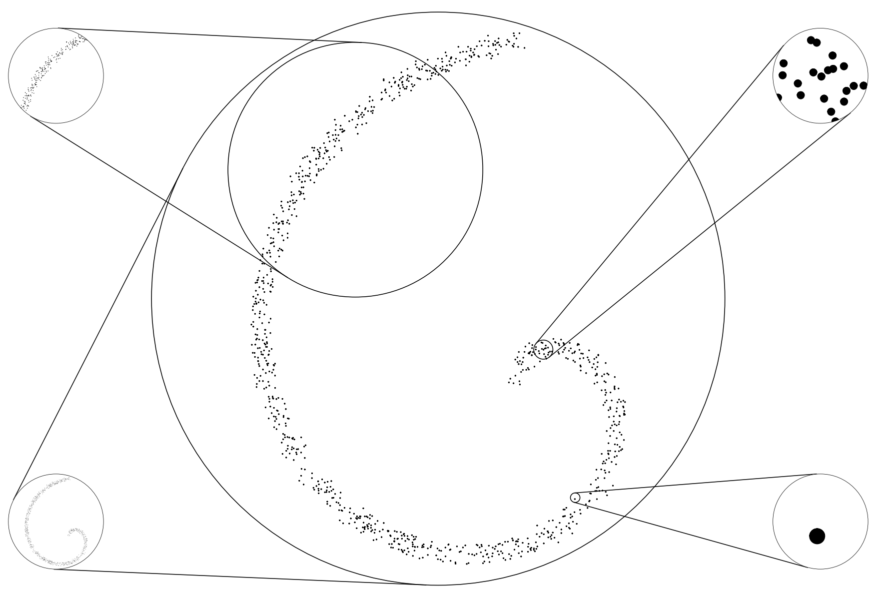
2020: Metric Space in Open Data

Correlation Dimension





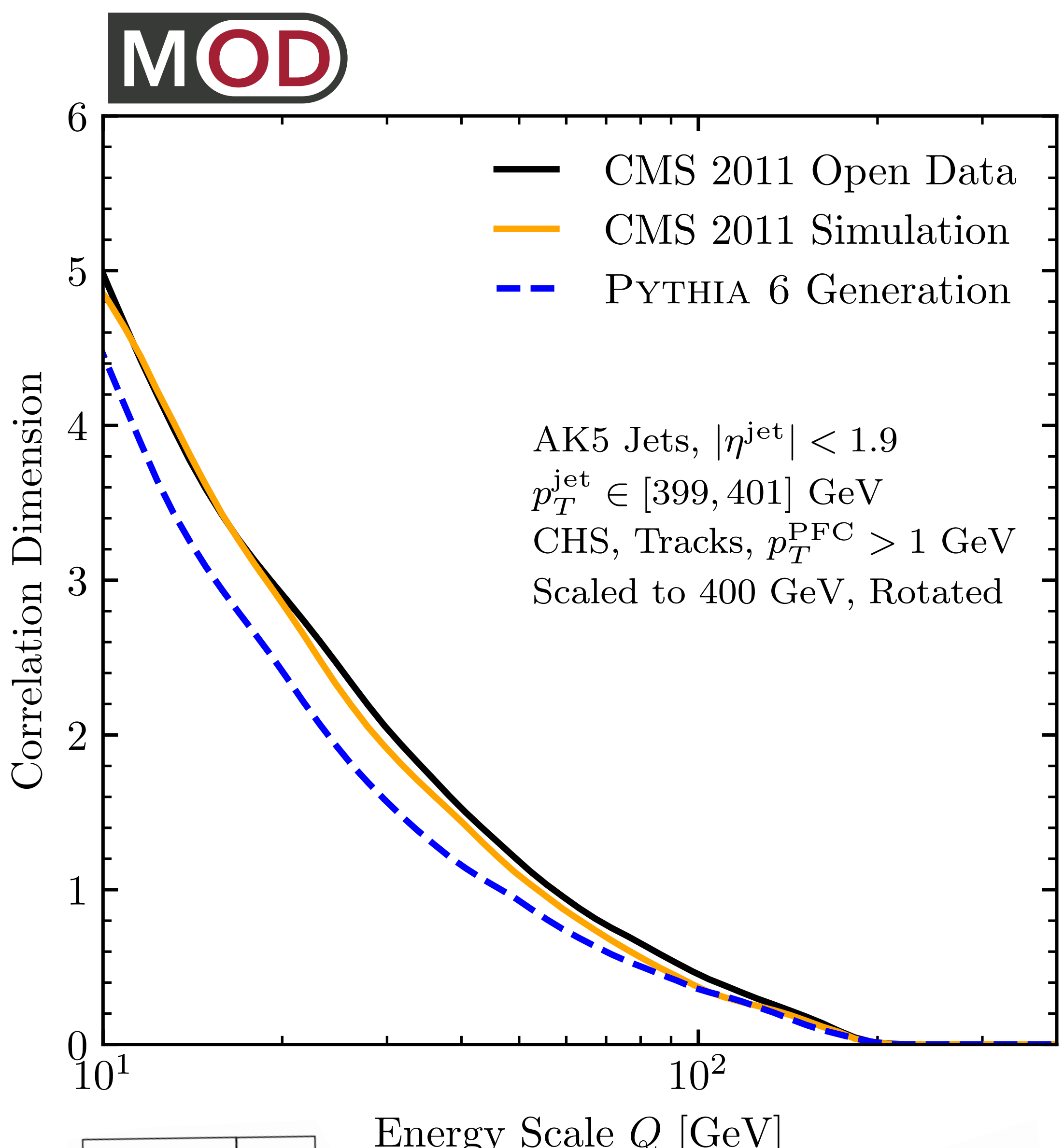
Scale-dependent dimension

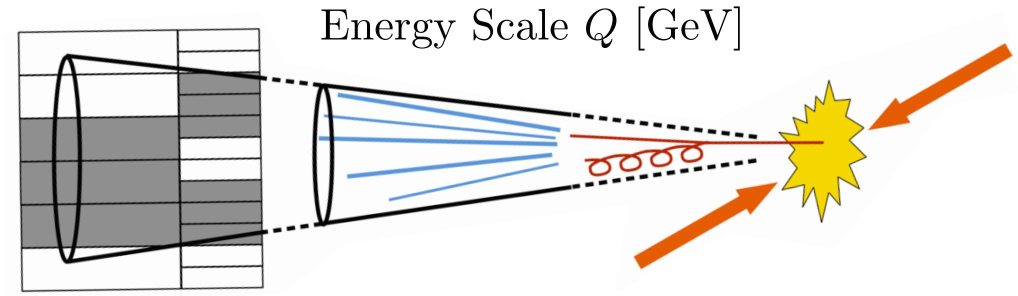


[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;
using Grassberger, Procaccia, PRL 1983; Kégl, NIPS 2002; using CMS Open Data]

2020: Metric Space in Open Data

Correlation Dimension





Scaling behavior of QCD!

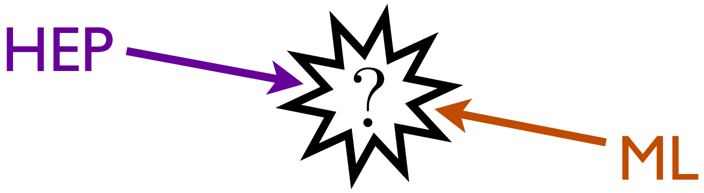
$$\mathrm{d}P_{i\to ig} \simeq \frac{2\alpha_s}{\pi} C_i \frac{\mathrm{d}\theta}{\theta} \frac{\mathrm{d}z}{z}$$

Hmm, detector effects distort underlying physics…

[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020; using Grassberger, Procaccia, PRL 1983; Kégl, NIPS 2002; using CMS Open Data]

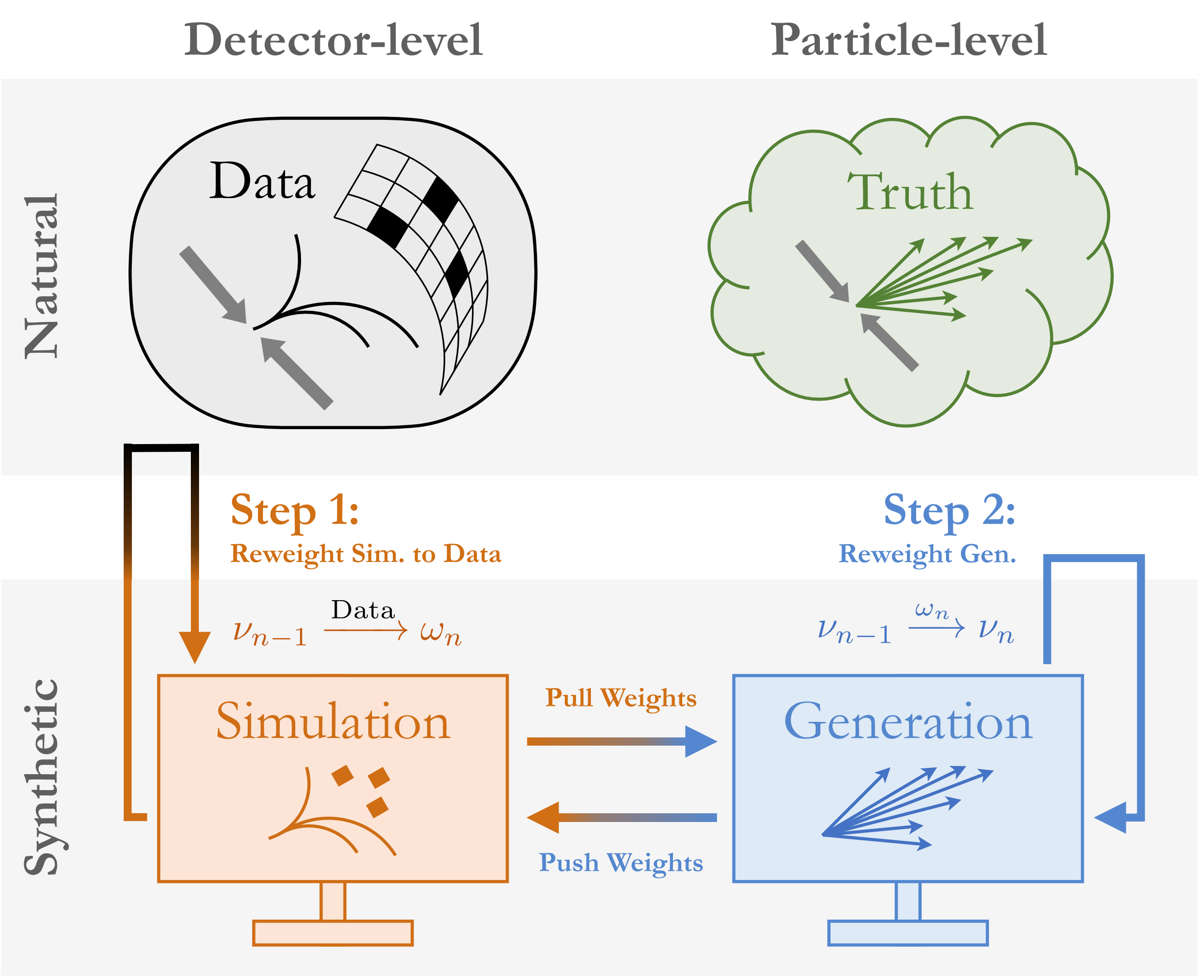
   

2020: Detector Unfolding

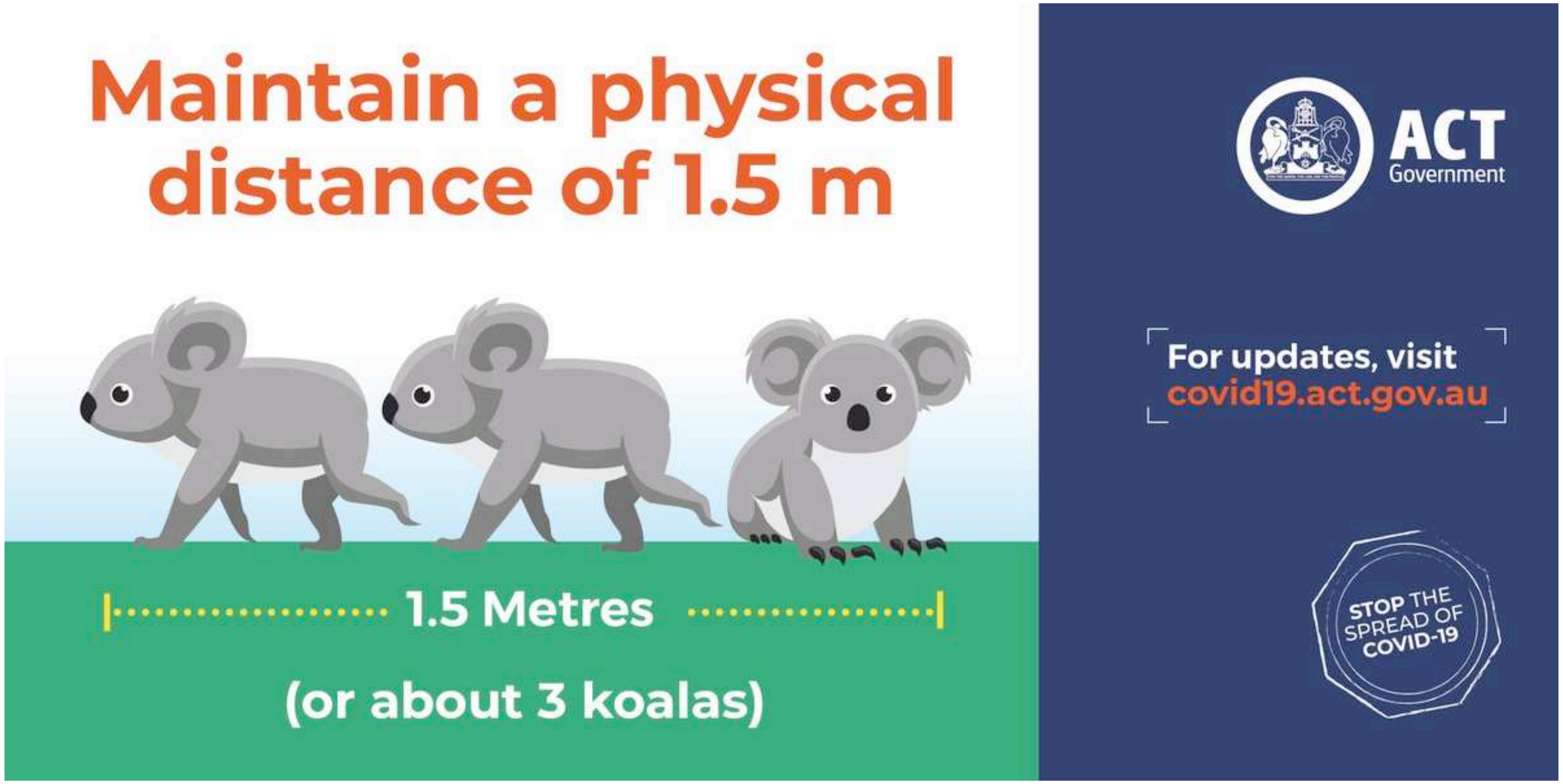


OmniFold

Multi-dimensional unbinned detector corrections via iterated application of machine-learned reweighting

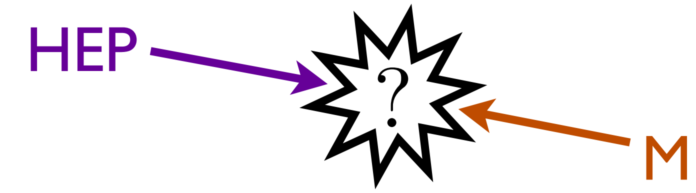


[Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020; + Suresh, ICLR SimDL 2021;
Komiske, McCormack, Nachman, PRD 2021; see unfolding comparison in Petr Baron, APPB 2021]
[see alternative in Bellagente, Butter, Kasieczka, Plehn, Rousselot, Winterhalder, Ardizzone, Köthe, SciPost 2020]

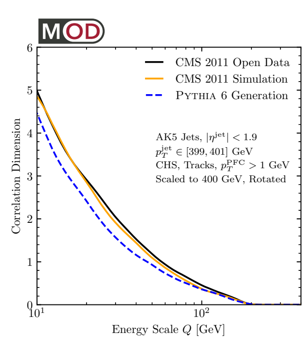

Maintain a physical distance of 1.5 m
1.5 Metres
(or about 3 koalas)
ACT Government
For updates, visit covid19.act.gov.au
STOP THE SPREAD OF COVID-19

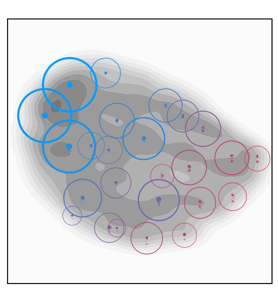
Oh, that…

2021: Launch of IAIFI

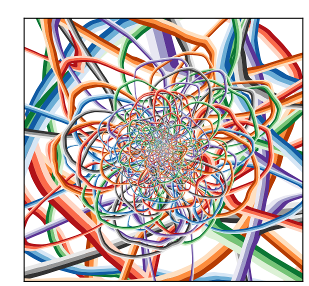


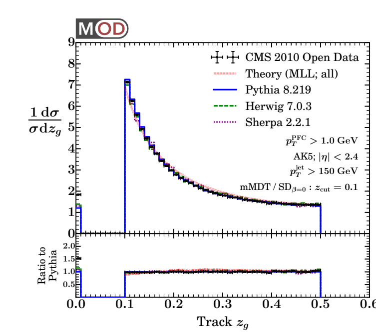
Can we finally put the "AI" in AItarelli-Parisi?





$$\mathrm{d}P_{i\to ig} \simeq \frac{2\alpha_s}{\pi} C_i \frac{\mathrm{d}\theta}{\theta} \frac{\mathrm{d}z}{z}$$

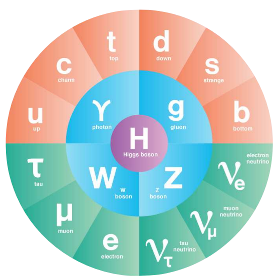




Must separate quarks from gluons!

2022: Putting All the Pieces Together

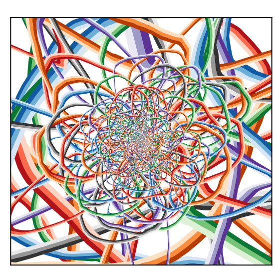
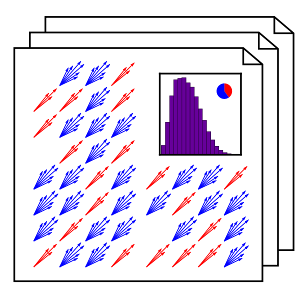

Quark and Gluon Jets from the Strong Force



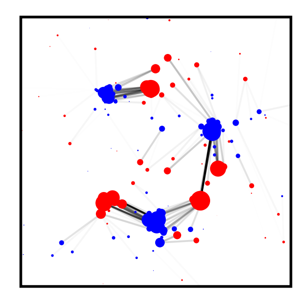
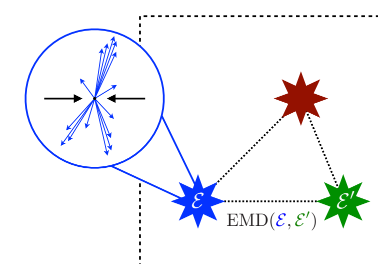
…Confronted with Public Collider Data…

…Unfolded for Detector Effects…

…Disentangled using Weak Supervision on Set-Based Classifiers with Topic Modeling…

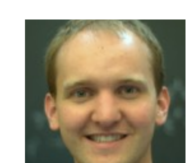
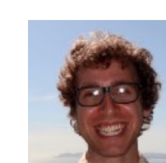




…Triangulated with Optimal Transport!

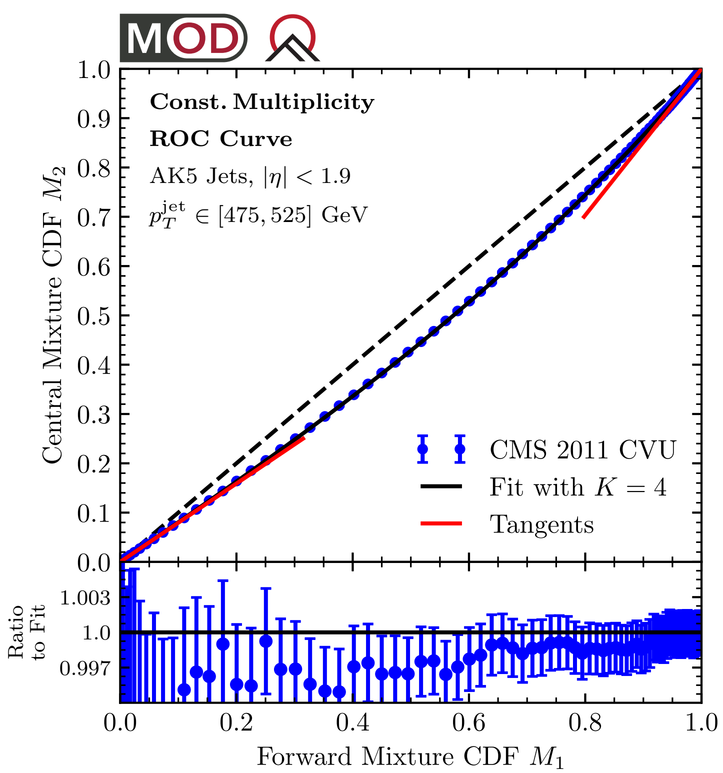
[Komiske, Kryhin, JDT, PRD 2022; using Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020; Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020; + Suresh, ICLR SimDL 2021; Metodiev, Nachman, JDT, JHEP 2017; Komiske, Metodiev, JDT, JHEP 2019; Metodiev, JDT, PRL 2018; Komiske, Metodiev, JDT, JHEP 2018; Komiske, Metodiev, JDT, PRL 2019]

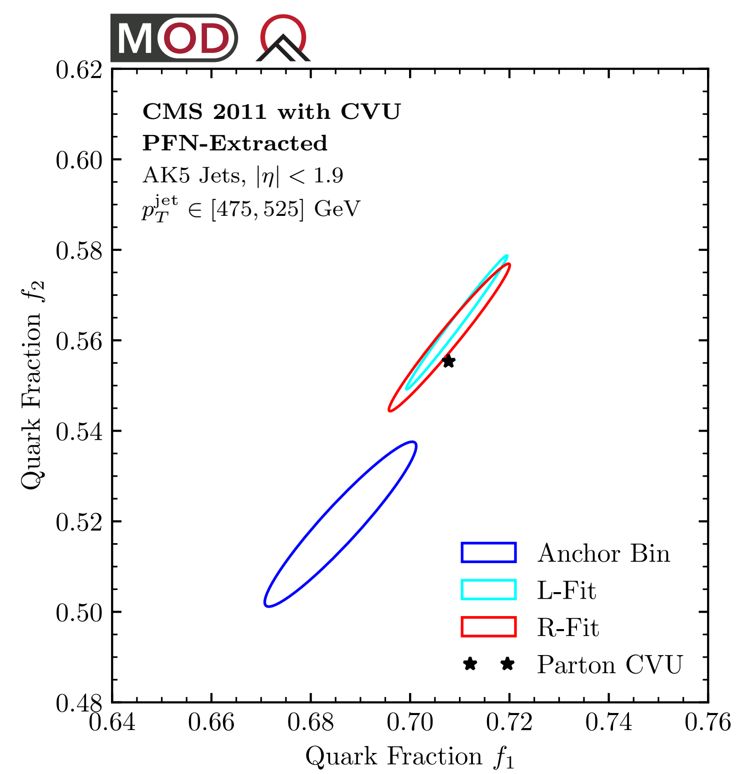


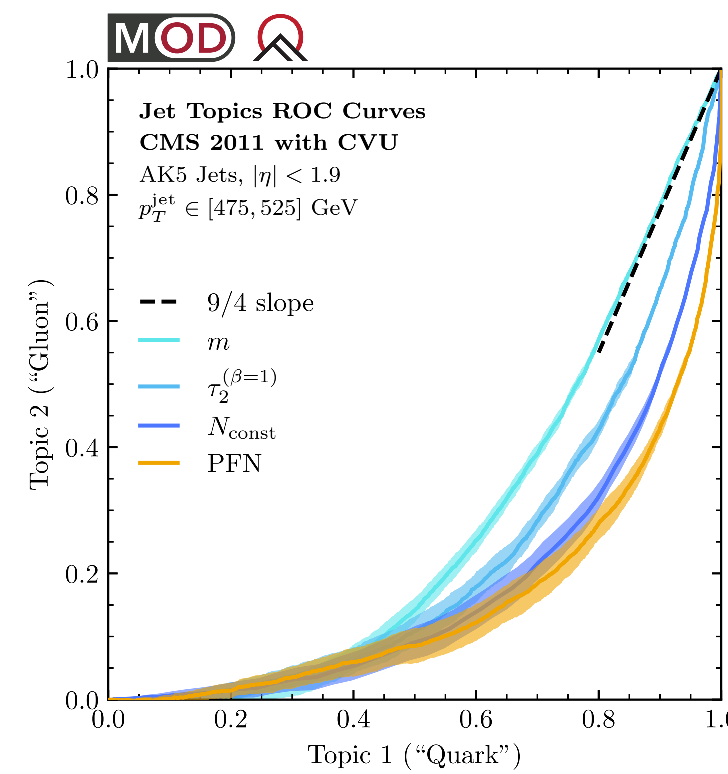




2022: Putting All the Pieces Together

Plus some technical details as to how we extract reducibility factors, determine correlated uncertainties, and validate the method…

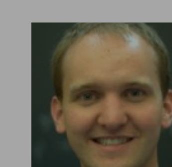


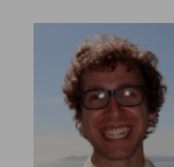




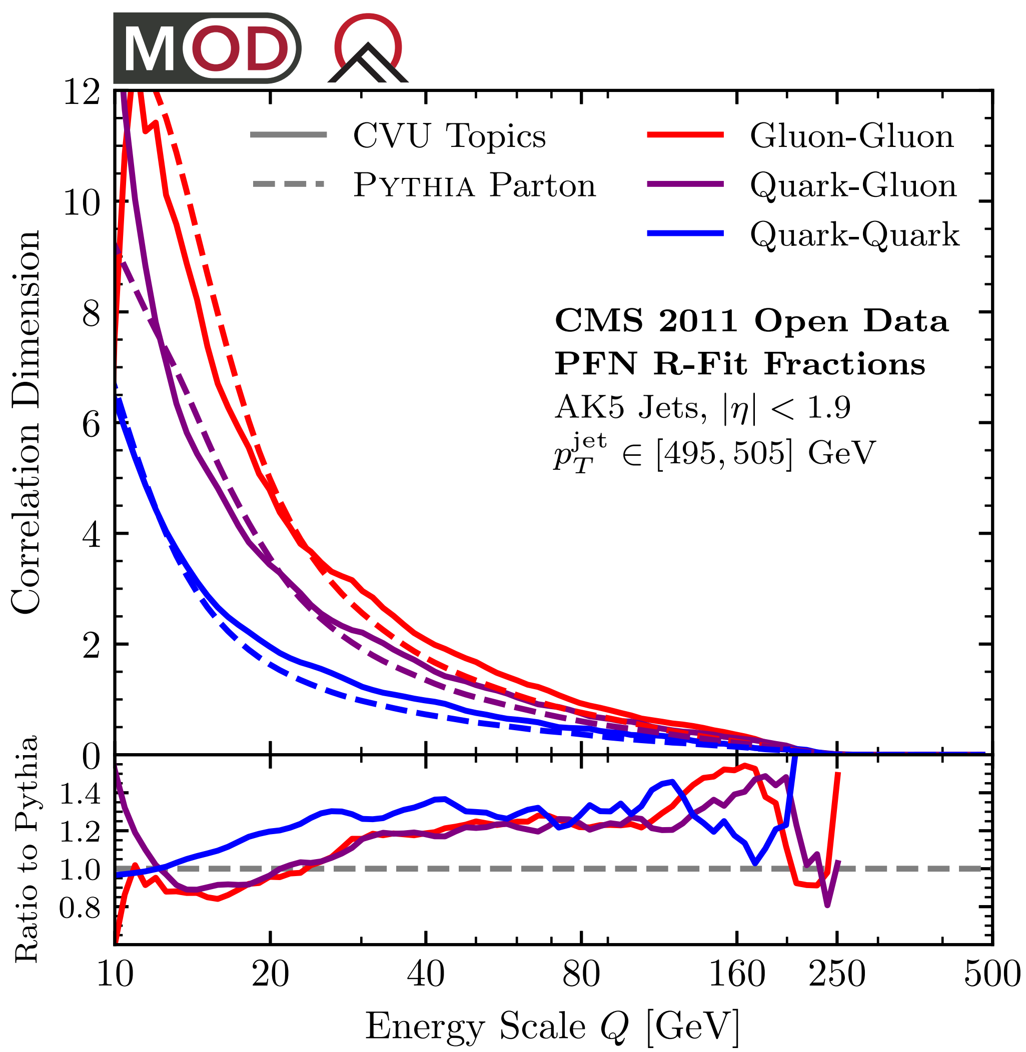
Once you know quark fractions, the rest is linear algebra

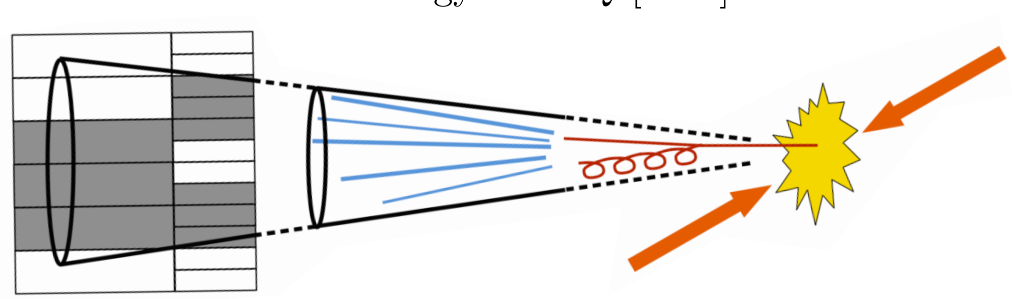
[Komiske, Kryhin, JDT, PRD 2022; using Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020; Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020; + Suresh, ICLR SimDL 2021; Metodiev, Nachman, JDT, JHEP 2017; Komiske, Metodiev, JDT, JHEP 2019; Metodiev, JDT, PRL 2018; Komiske, Metodiev, JDT, JHEP 2018; Komiske, Metodiev, JDT, PRL 2019]

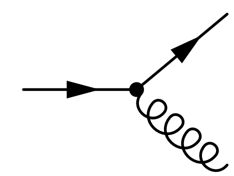




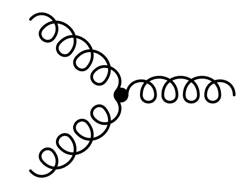
Dimensionality of Quark/Gluon Jets







First Principles QCD Calculation:



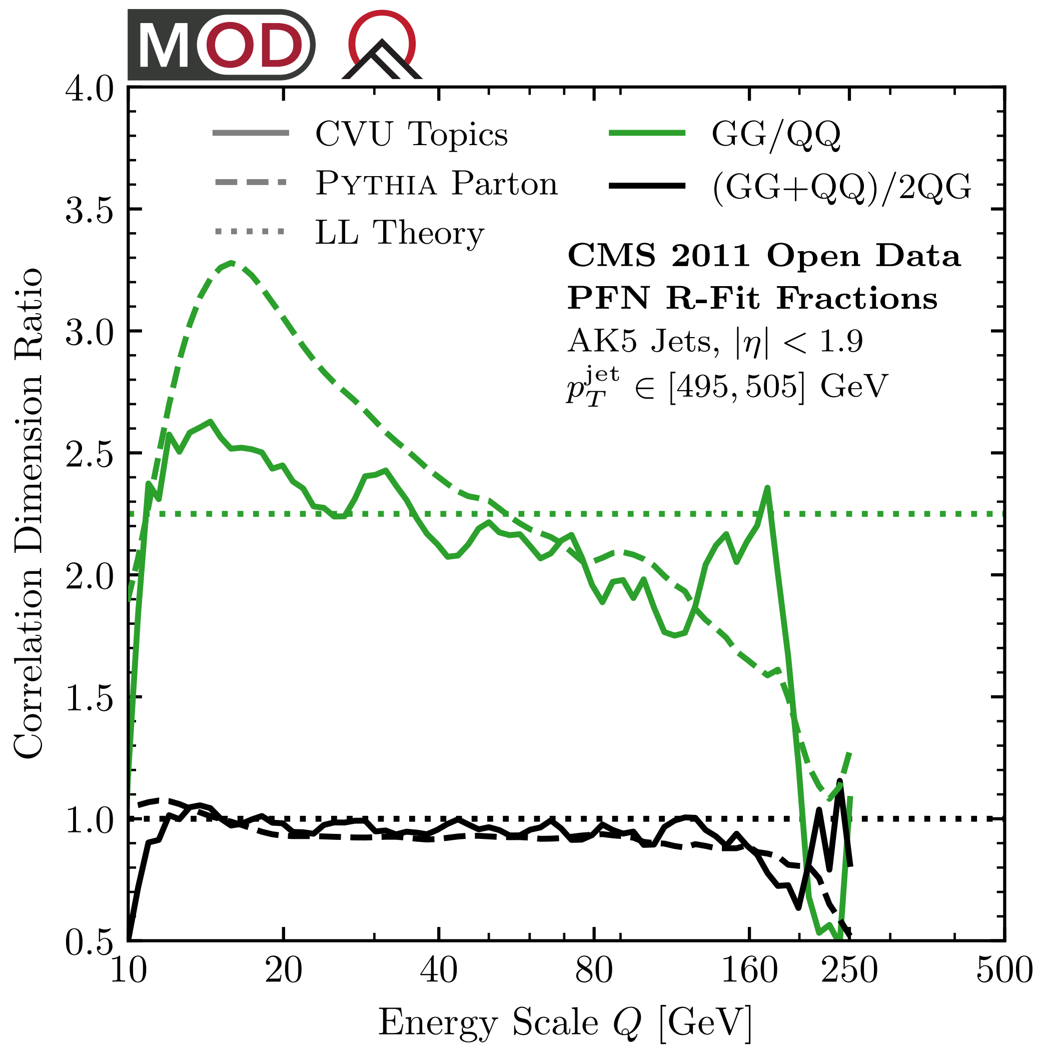
$$\dim_{IJ}(Q) \simeq \frac{2\alpha_s}{\pi}\left(C_I + C_J\right)\ln\frac{p_T/2}{Q}$$

Color Factors of QCD!

$$\mathrm{d}P_{i\to ig} \simeq \frac{2\alpha_s}{\pi} C_i \frac{\mathrm{d}\theta}{\theta}\frac{\mathrm{d}z}{z}$$

[Komiske, Kryhin, JDT, PRD 2022]

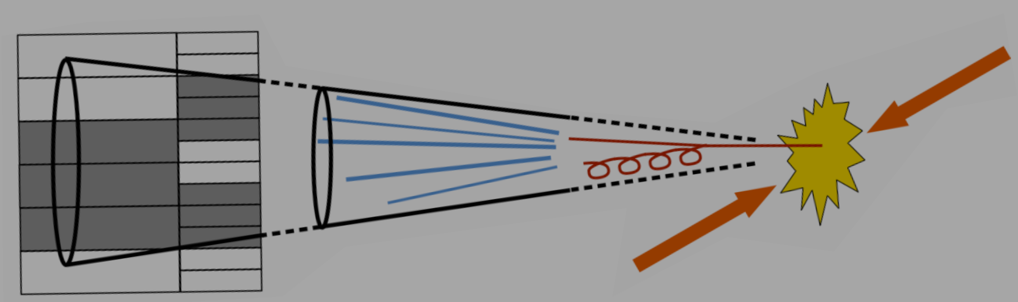
Dimensionality of Quark/Gluon Jets



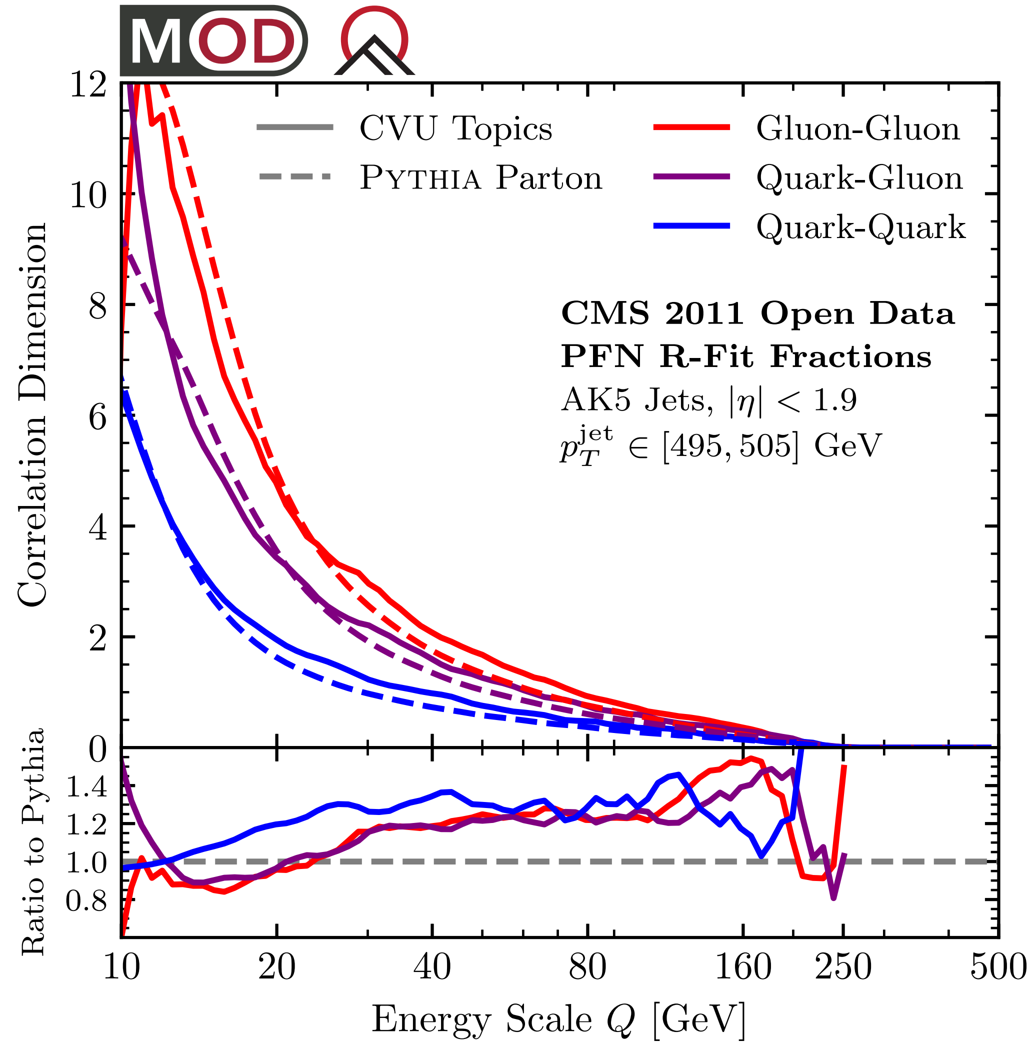
Fully data-driven extraction of quark/gluon color ratio

$$\frac{9}{4} = \frac{3}{4/3}$$

$$1 = \frac{(3) + (4/3)}{(3 + 4/3)}$$

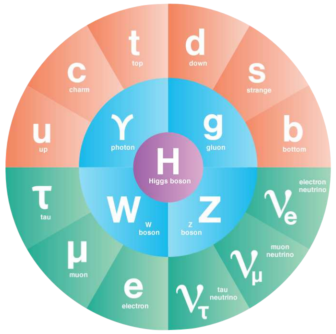


[Komiske, Kryhin, JDT, PRD 2022]



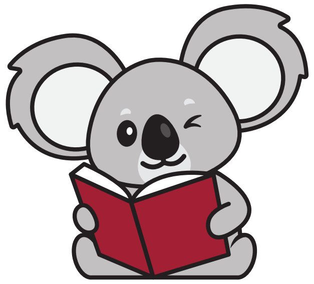
We gained new insights into strong force by fusing advances in machine learning with insights from quantum field theory

Summary



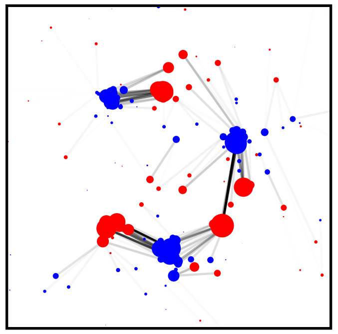
2017: A Quark/Gluon Conundrum

Quark/gluon jets offer an extreme example where fully supervised learning is fundamentally ambiguous



2018: Leveraging Weak Supervision

Assuming that "quark" and "gluon" jet categories exist, one can use machine learning to operationally define them

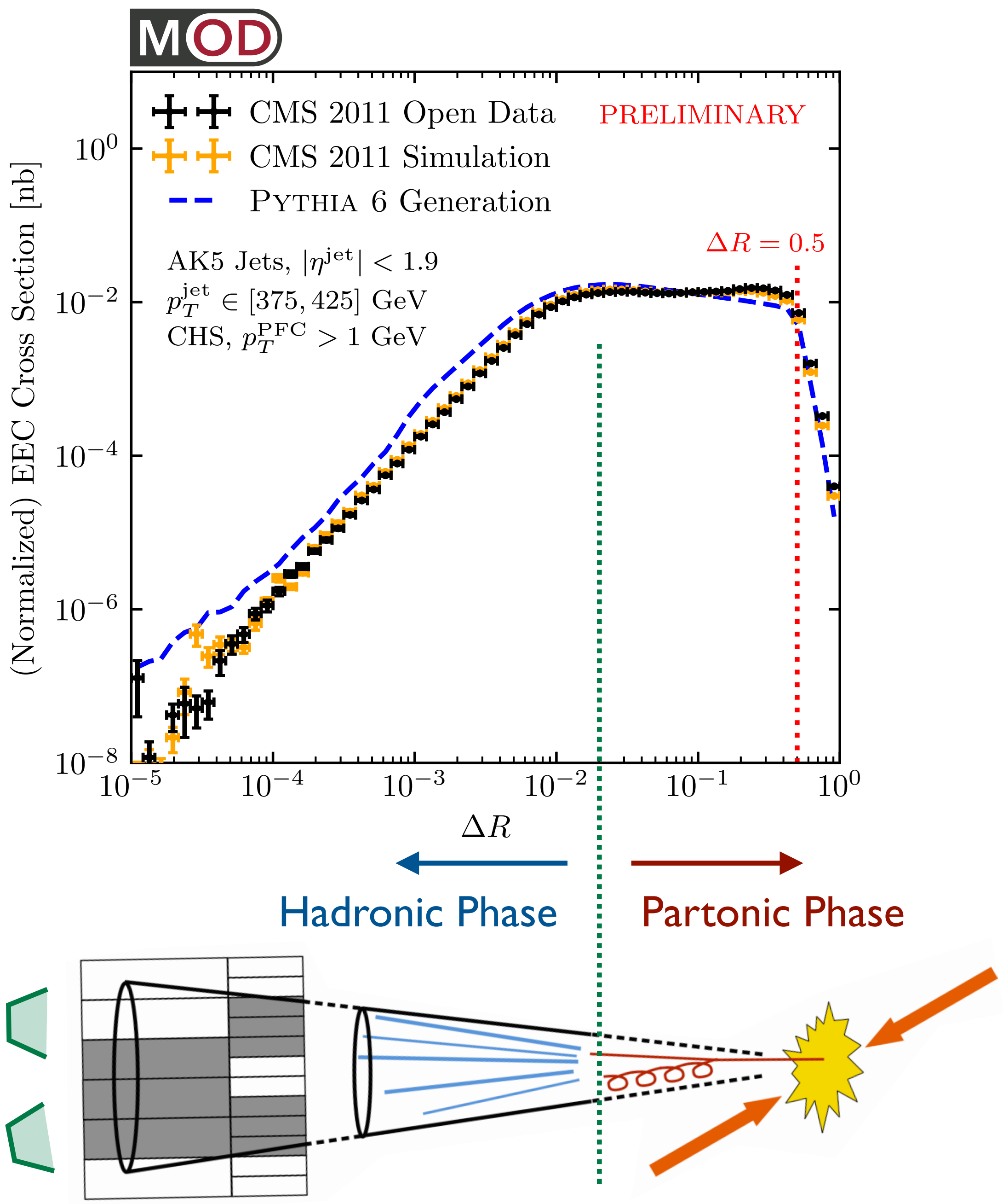


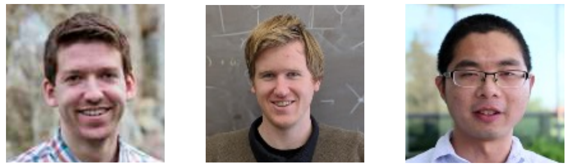
2019-2022: The Strong Force Revisited

Jet physics has crossed a important threshold where machine learning is now yielding insights that go beyond traditional analysis techniques

Backup Slides

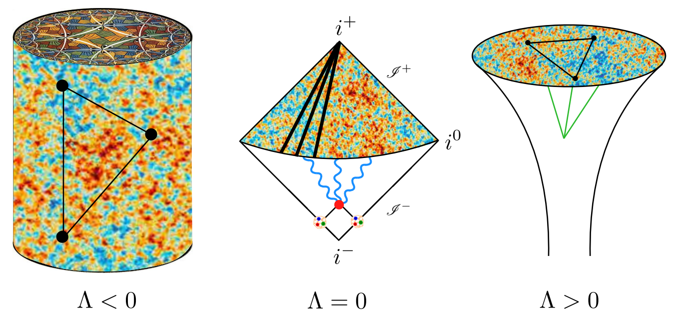
QCD through the Lens of Condensed Matter

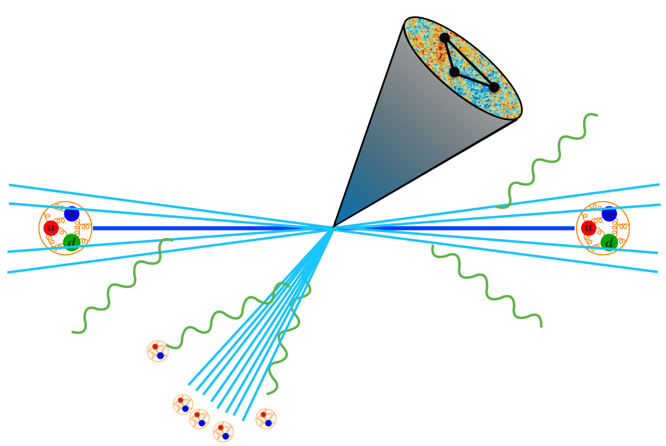


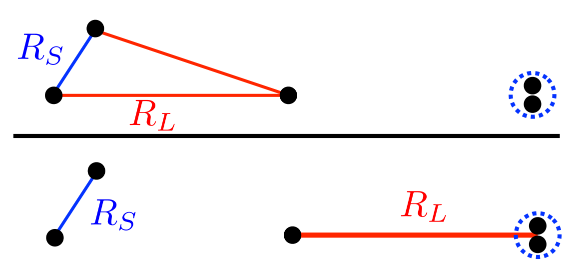


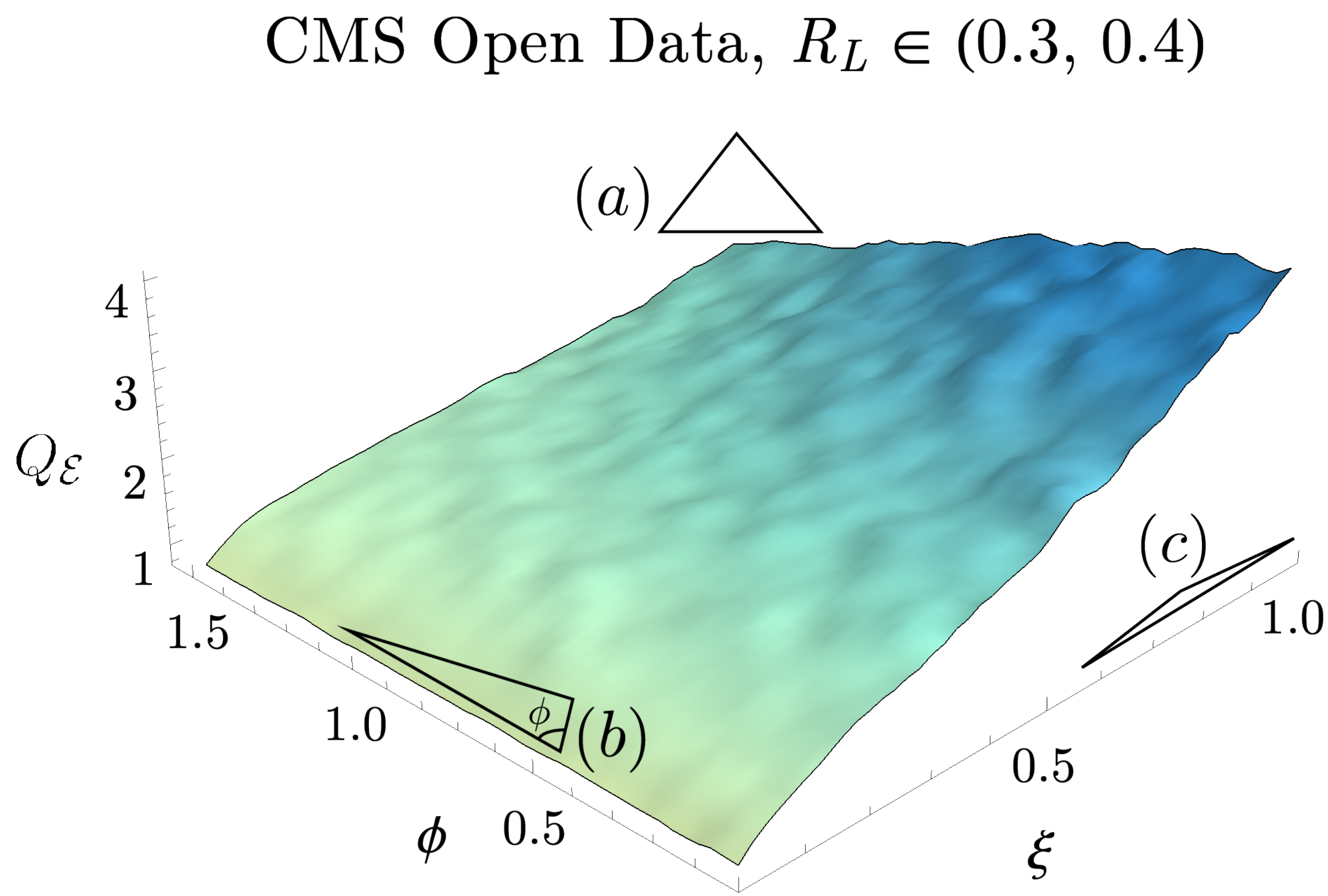
[Komiske, Moult, JDT, Zhu, arXiv 2022; see talks by Moult, BOOST 2019, BOOST 2020]

QCD through the Lens of Cosmology

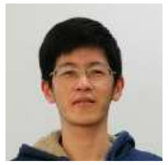
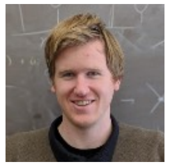
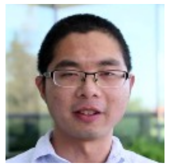








[Chen, Moult, JDT, Zhu, JHEP 2022]

Patrick Komiske

Eric Metodiev

Principles of Fundamental Physics

Robustness of Energy Flow

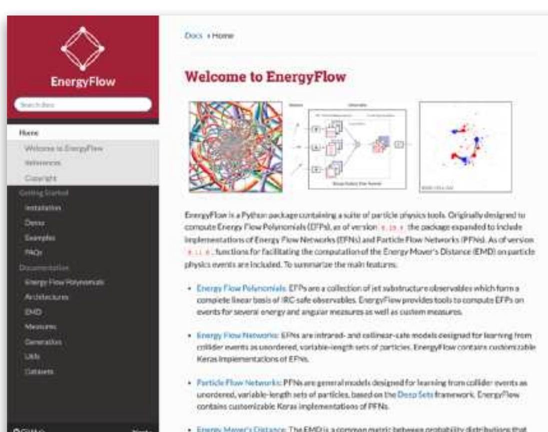
[Komiske, Metodiev, JDT, JHEP 2018]

?

Power of Artificial Intelligence

Point Cloud Learning

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

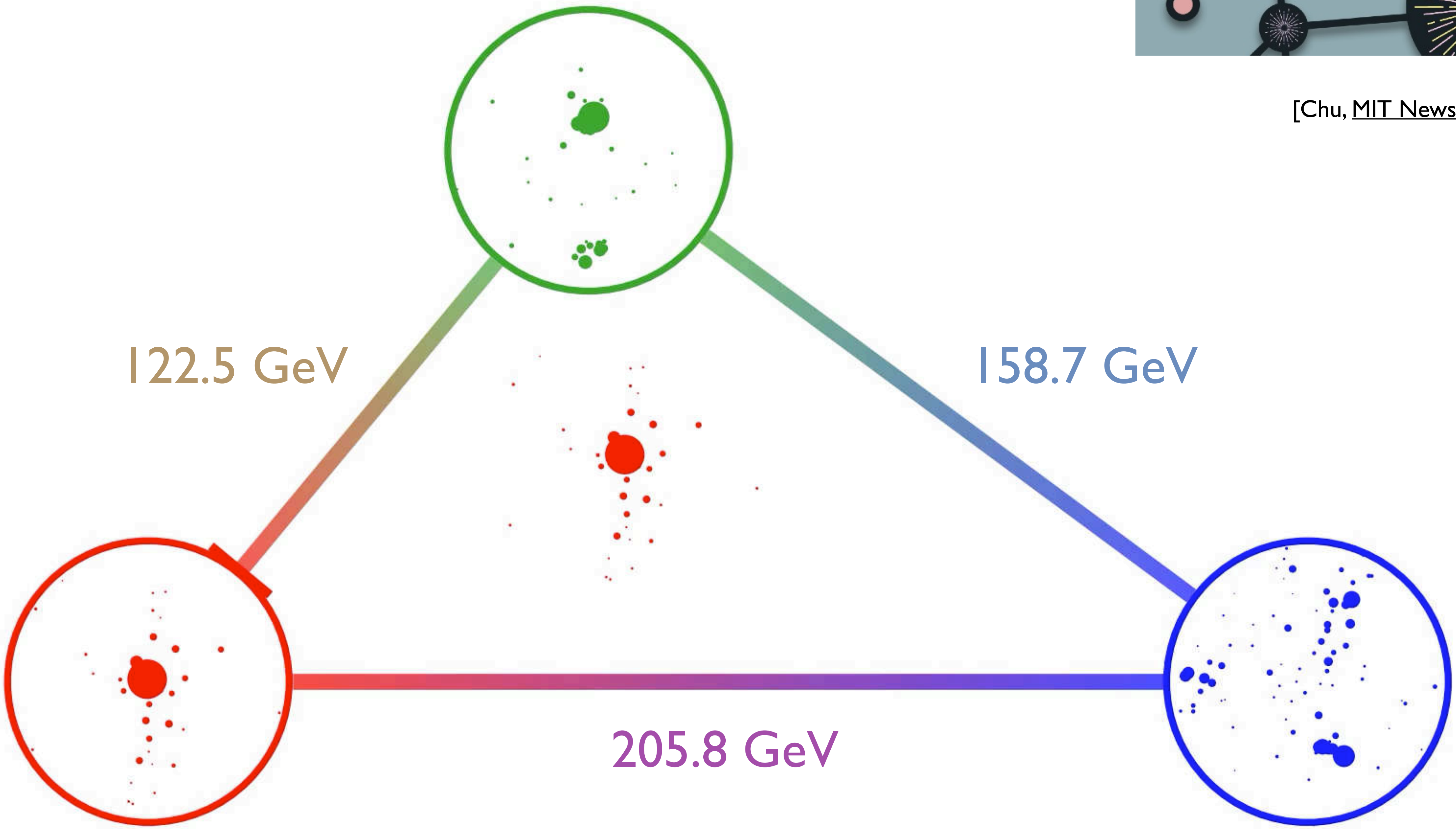


Energy Flow Networks

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

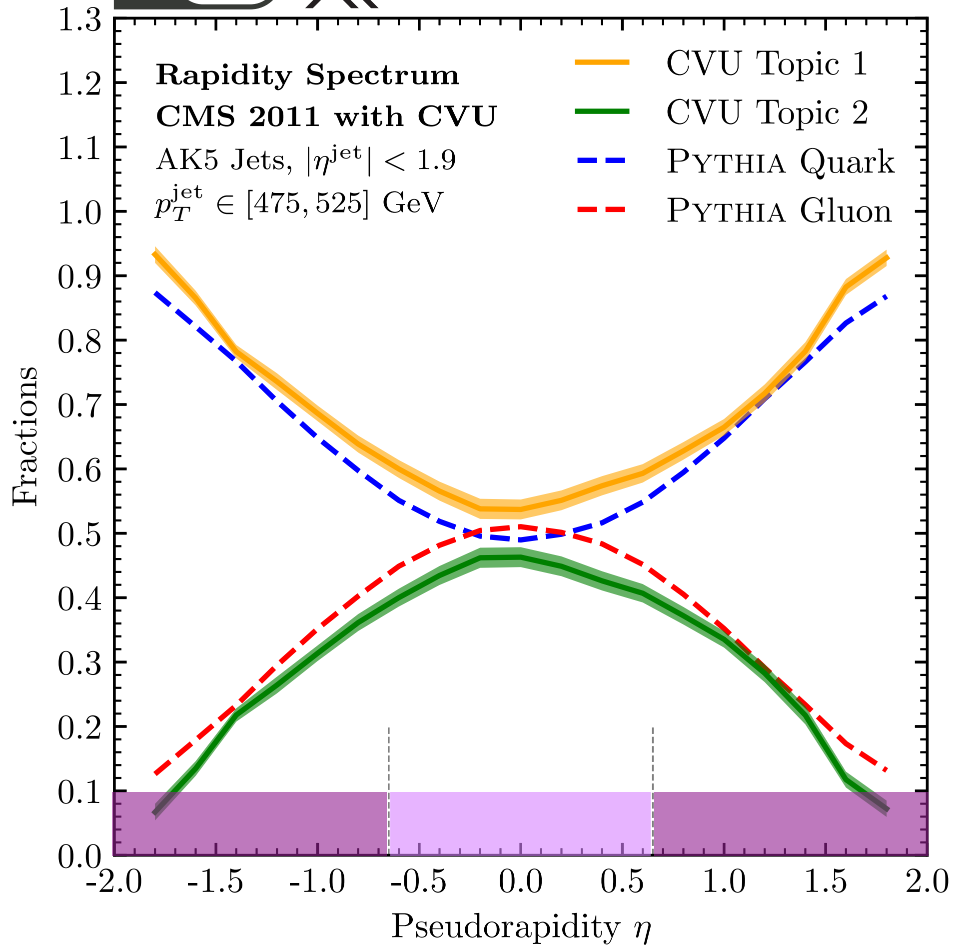
Triangulating the Space of Jets

[Chu, MIT News July 2019]

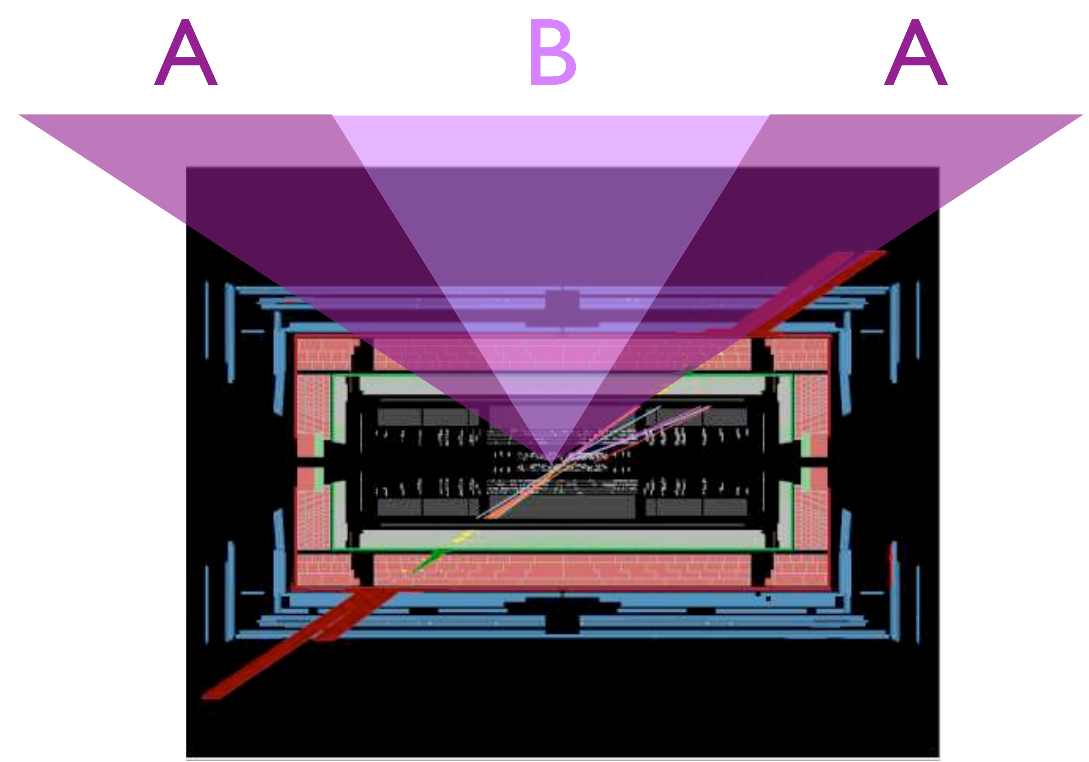


[Komiske, Metodiev, JDT, PRL 2019; code at Komiske, Metodiev, JDT, energyflow.network; see alternative graph network approach in Mullin, Pacey, Parker, White, Williams, JHEP 2021]

Rapidity-Dependent Quark/Gluon Fraction



A B A



[Komiske, Kryhin, JDT, arXiv 2022]

Likelihood Ratio Trick

Many HEP 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): $L = -\langle \log f(x) \rangle_P + \langle f(x) - 1 \rangle_Q$

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

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

[see e.g. Cranmer, Pavez, Louppe, arXiv 2015; D'Agnolo, Wulzer, PRD 2019;
simulation-based inference in Cranmer, Brehmer, Louppe, PNAS 2020;
relation to f-divergences in Nguyen, Wainwright, Jordan, AoS 2009; Nachman, Thaler, PRD 2021]

Likelihood Ratio Trick

Key example of simulation-based inference

Many HEP 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. Cranmer, Pavez, Louppe, arXiv 2015; D'Agnolo, Wulzer, PRD 2019;
simulation-based inference in Cranmer, Brehmer, Louppe, PNAS 2020;
relation to f-divergences in Nguyen, Wainwright, Jordan, AoS 2009; Nachman, Thaler, PRD 2021]

Machine Learning Requirements

If you have in hand…

Well-specified loss
Reliable training data
Learnable function

…then you can leverage ML!

Many HEP tasks can be phrased in this language

Physics input essential for robust usage of these tools

[see HEPML-LivingReview for extensive bibliography]