

Collision Course

Particle Physics meets Machine Learning

Jesse Thaler



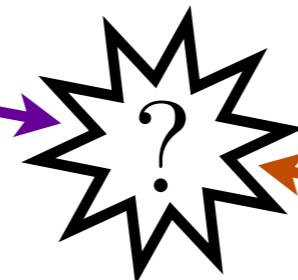
Google X, Tech Talk — April 15, 2019

“Collision Course”

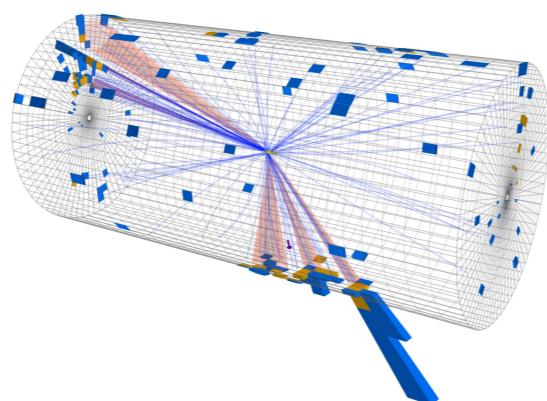
“*Theoretical Physics for Machine Learning*”
Aspen Center for Physics, January 2019

(Theoretical)
Particle
Physics

Mathematics,
Statistics,
Computer Science



Could



be the next

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?

My Perspective c. 2016



“Deep Learning” vs. “Deep Thinking”

My Perspective c. 2018



“Deep Learning” & vs. “Deep Thinking”

“Deep Learning” *is*
 ~~&~~ “Deep Thinking”
 ~~vs.~~

*New insights into fundamental physics
facilitated by advances in
mathematics, statistics, and computer science*

(and vice versa)

Proximate Reasons for My Conversion



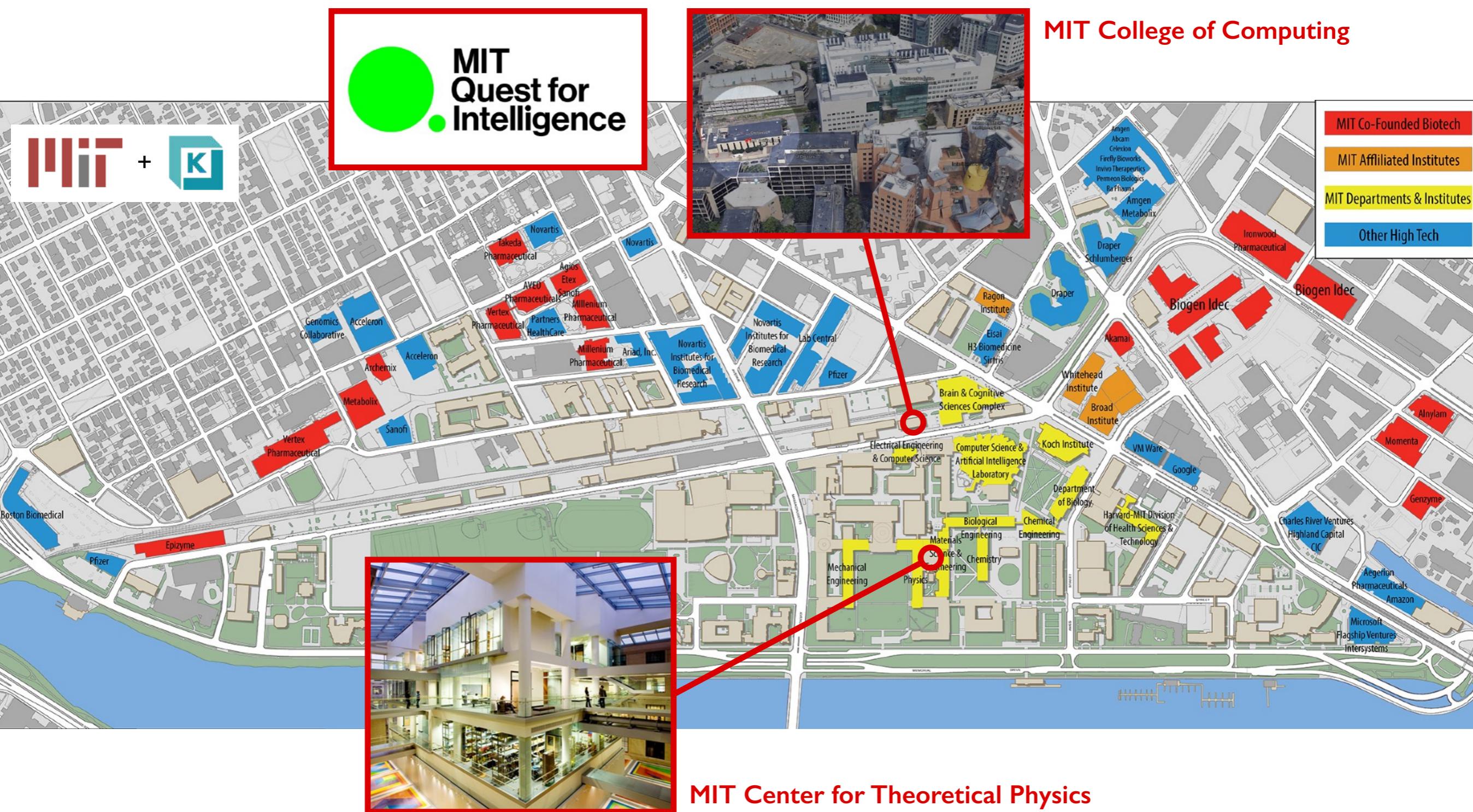
Patrick Komiske



Eric Metodiev

plus Ben Nachman, Kyle Cranmer, Daniel Whiteson, Mike Williams, Matt Schwartz, Dan Roberts, Phiala Shanahan, ...

Proximate Reasons for Sustained Excitement



(Even more than this; map from 2014)

Ultimate Goal

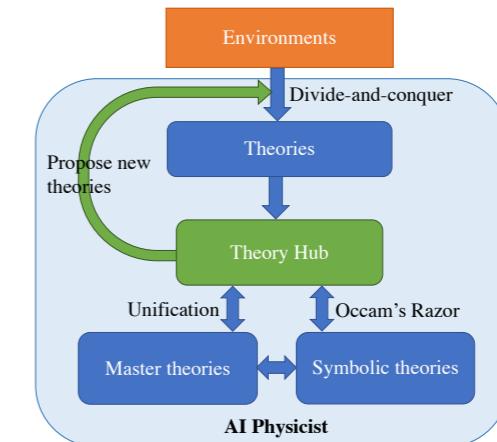
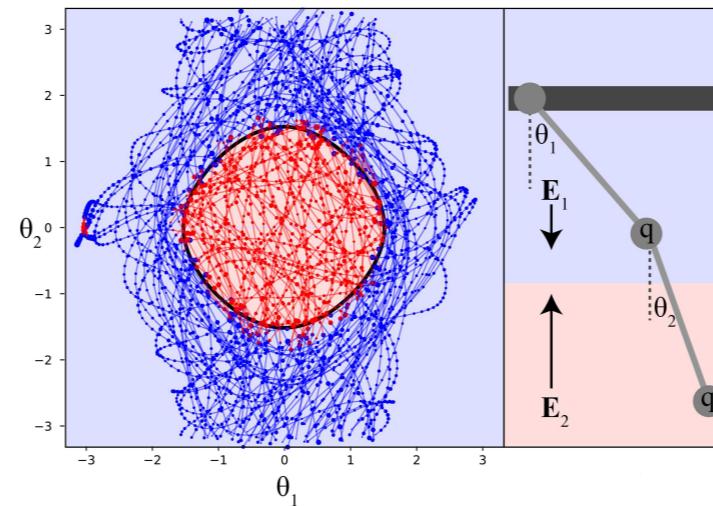
Teach a Machine to “Think like a Physicist”

(really, any scientist)

As opposed to “Learn like a Toddler”
Have you ever tried to reason with a 2 year old?

AI-saac Newton?

[e.g. Wu, Tegmark, [1810.10525](#)]



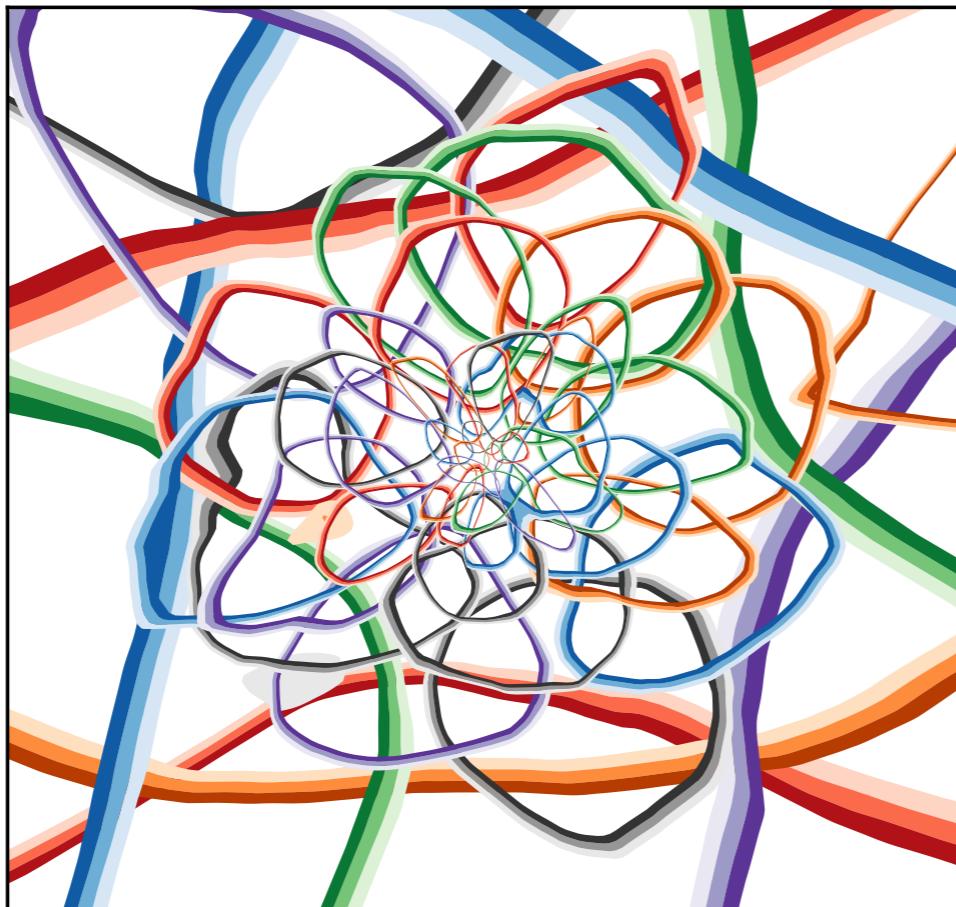
Physics 8.01

1. Specify the problem ← True creative intelligence
2. Find the solution ← ML does amazingly well
3. Verify the solution ← ML can get in the way

Today's Goal

Teach a Machine to Communicate to a Physicist

As opposed to trying to reverse engineer a
black box machine learning architecture



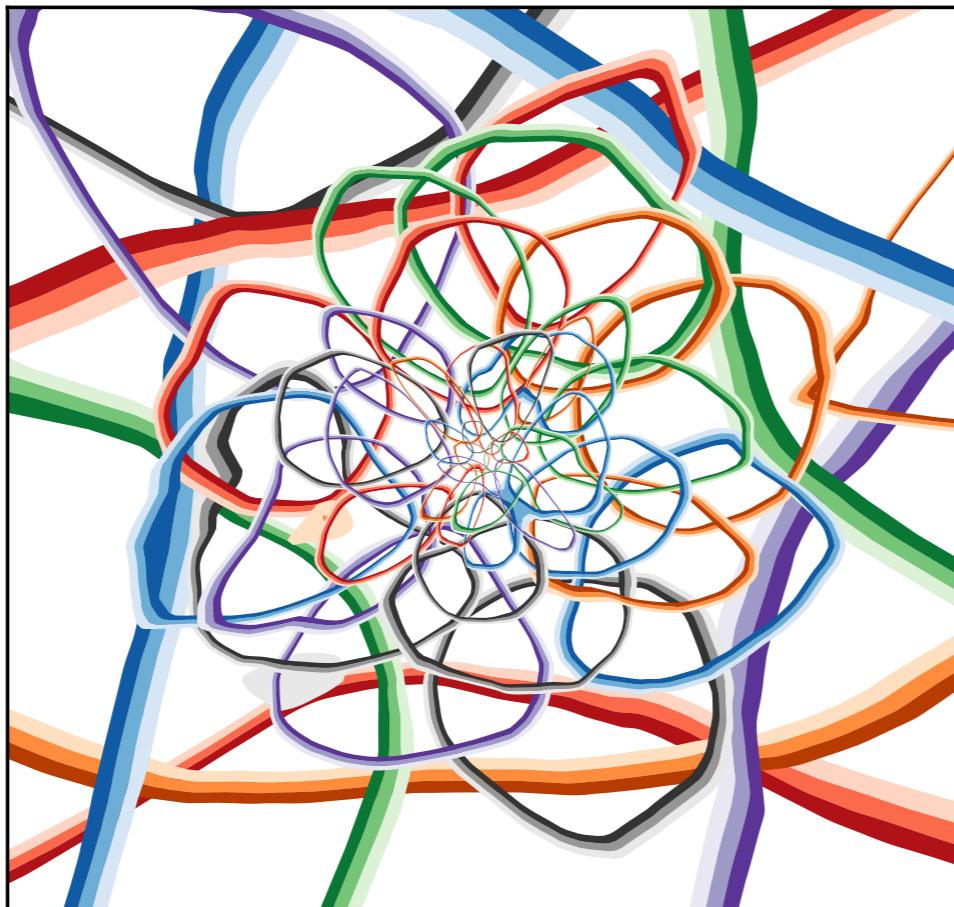
**Learning the
Altarelli-Parisi
splitting kernel**

[Komiske, Metodiev, JDT, [1810.05165](#)]

Today's Goal

Teach a Machine to Communicate to a Physicist

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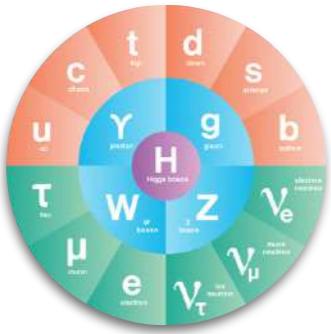


Learning the
Altarelli-Parisi
splitting kernel

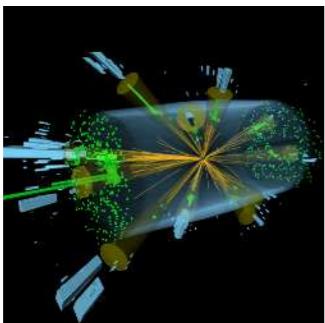
(without us asking it to!)

[Komiske, Metodiev, JDT, [1810.05165](#)]

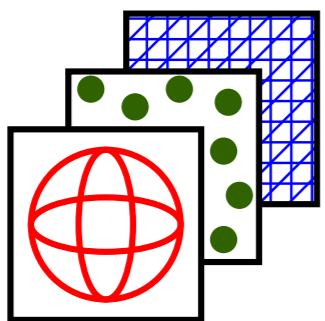
Outline



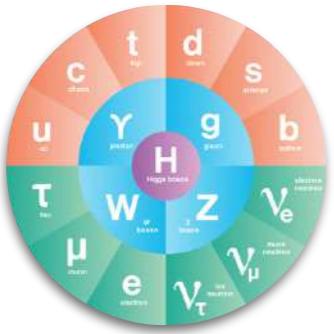
Particle Physics Primer



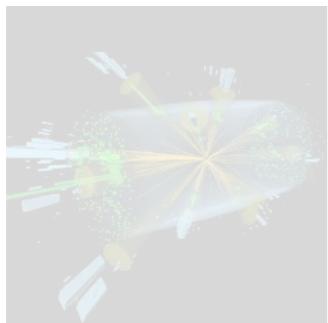
Jets and Point Clouds



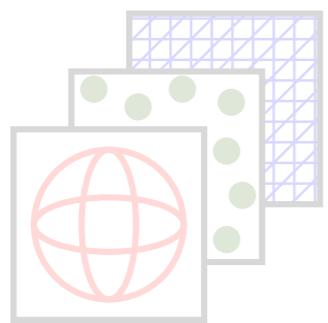
Energy Flow Networks



Particle Physics Primer

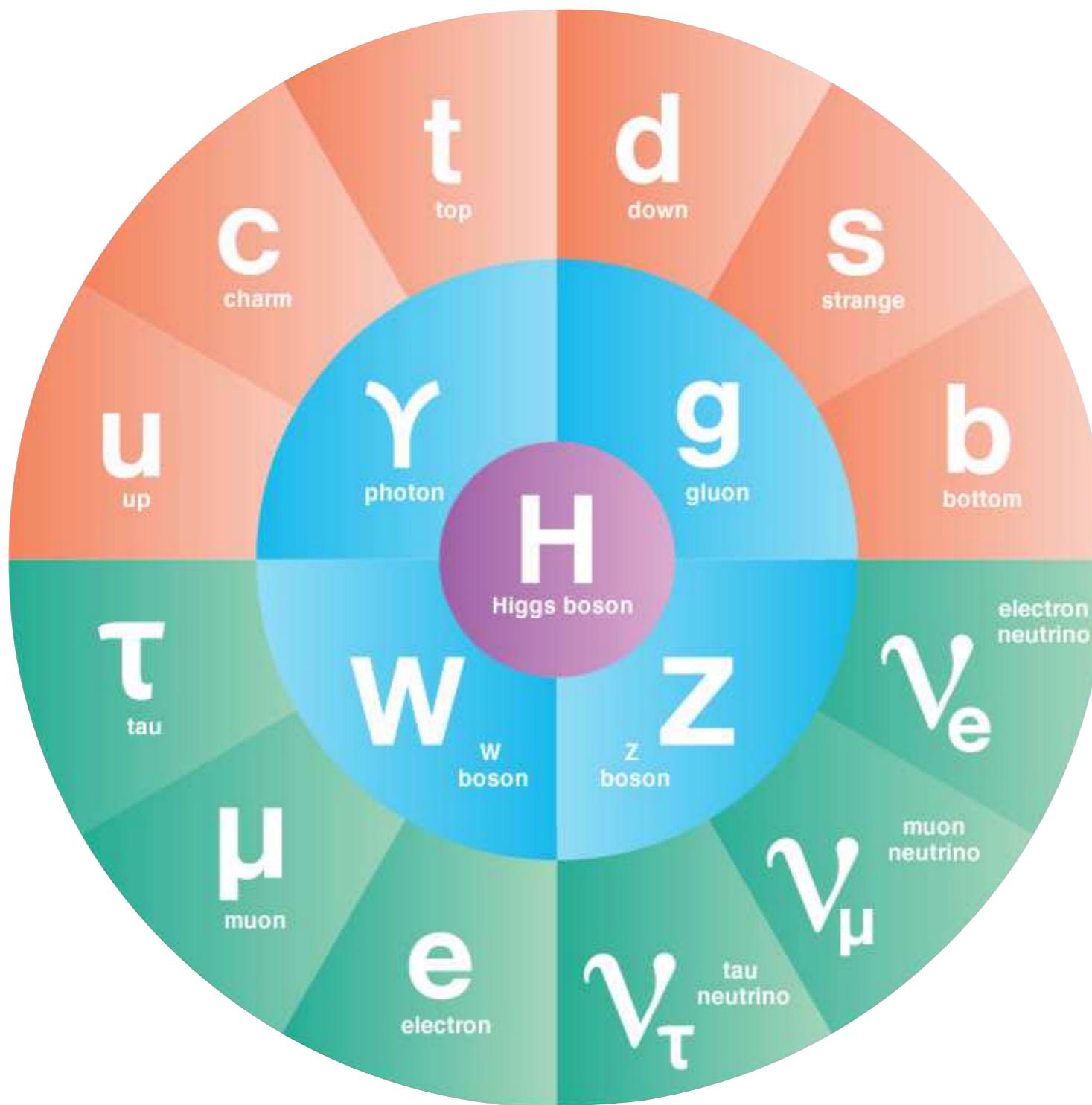


Jets and Point Clouds

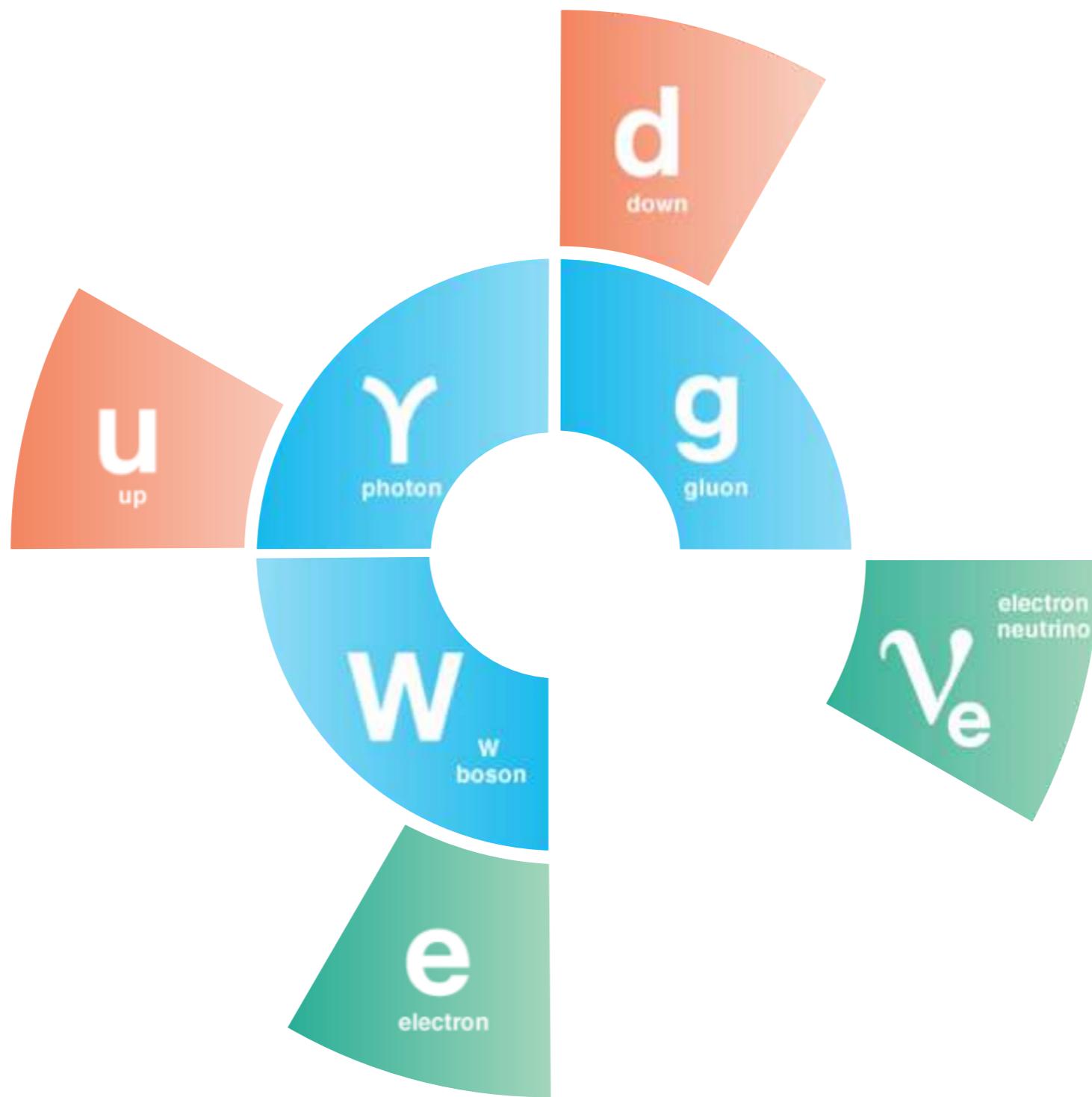


Energy Flow Networks

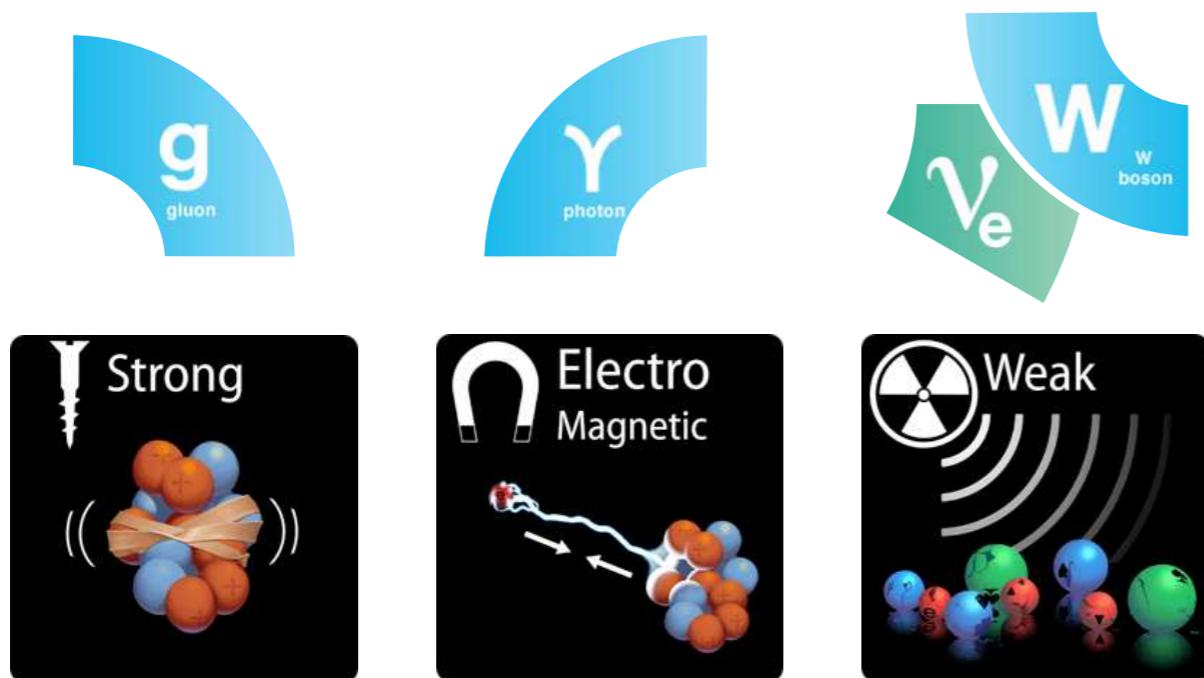
The Standard Model



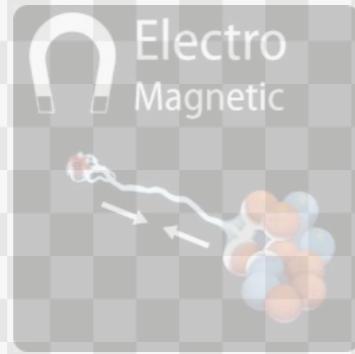
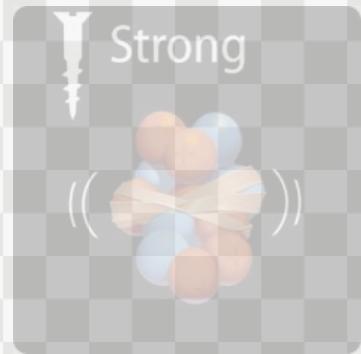
Ordinary Matter



Ordinary Matter



Dark Matter (& Dark Energy)

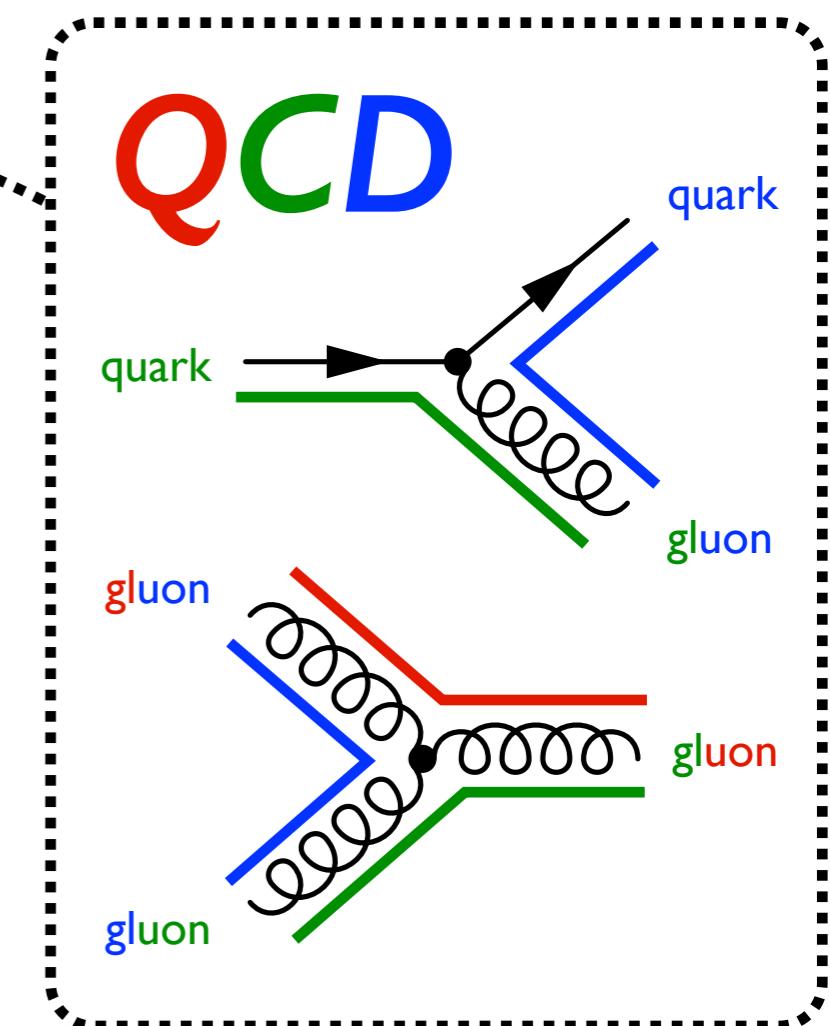
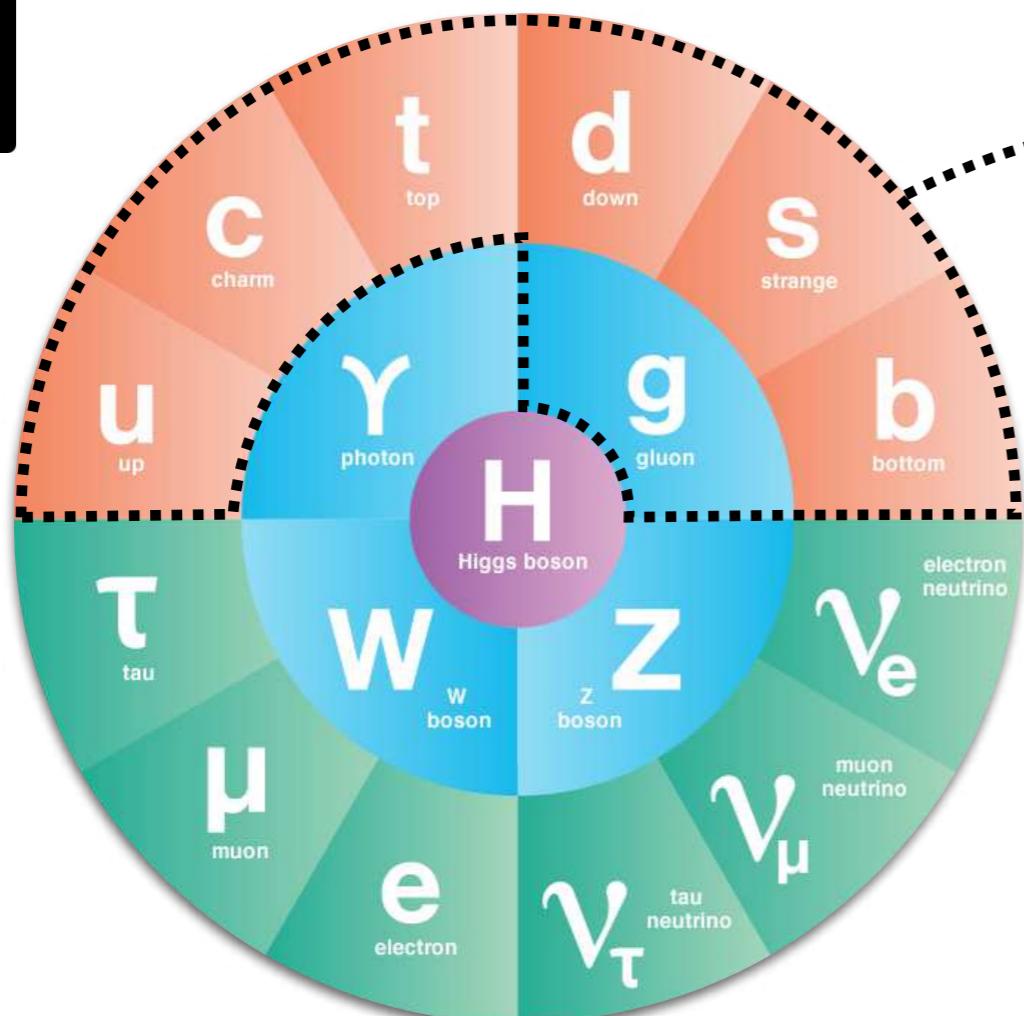
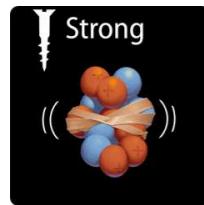


Dark Forces?

A dashed arrow points from the text "Dark Forces?" to the fourth icon.

Focus on the Strong Force

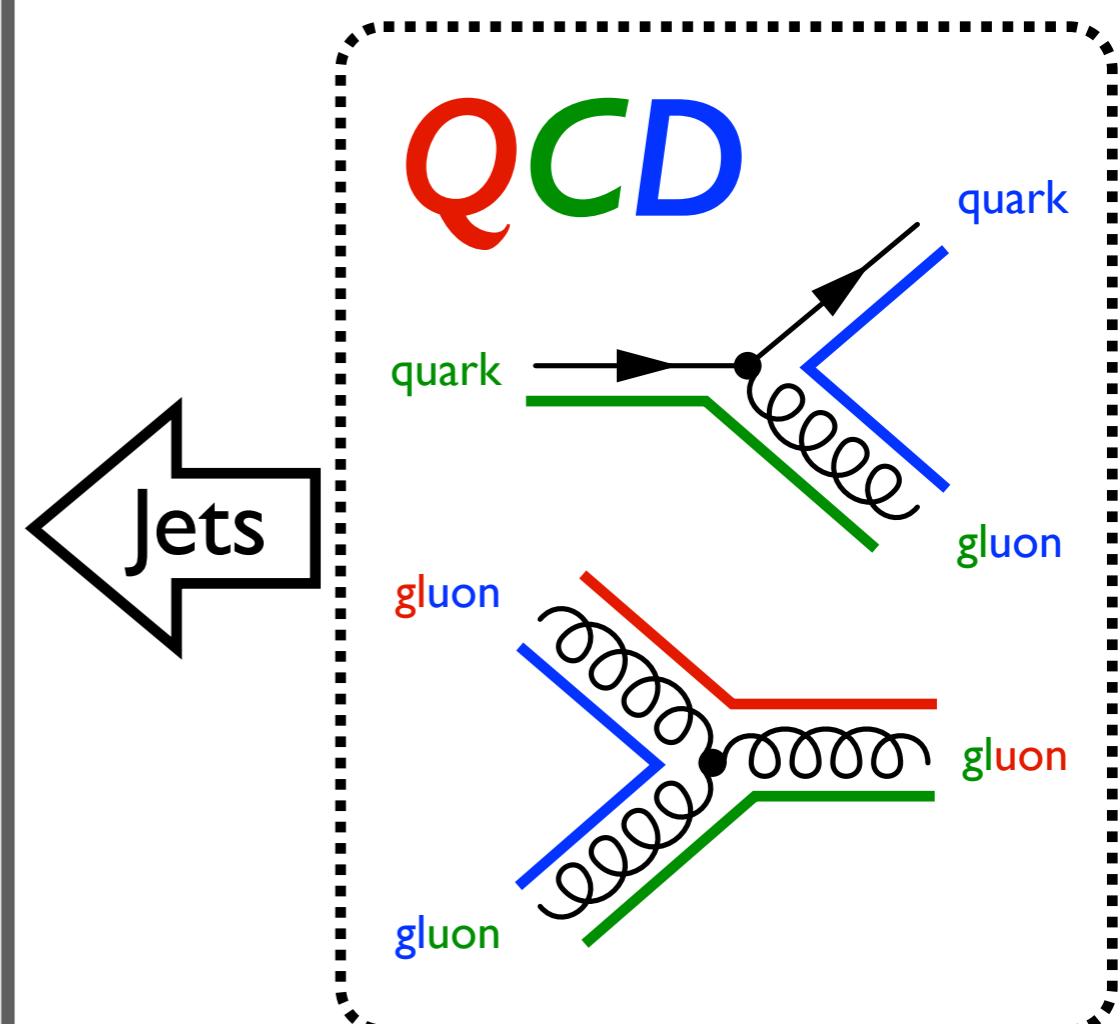
Crucial for physics at the Large Hadron Collider

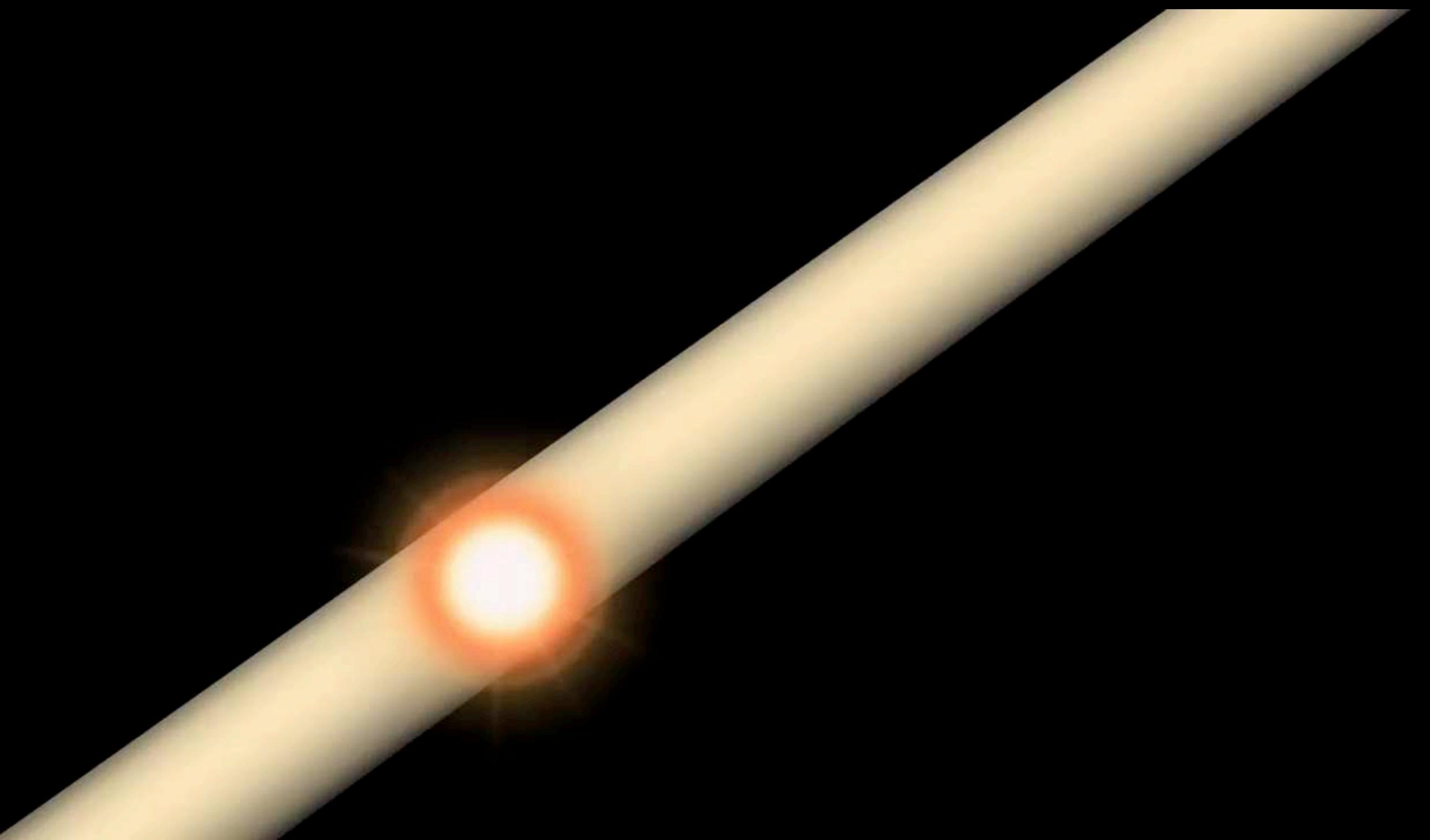


Focus on the Strong Force

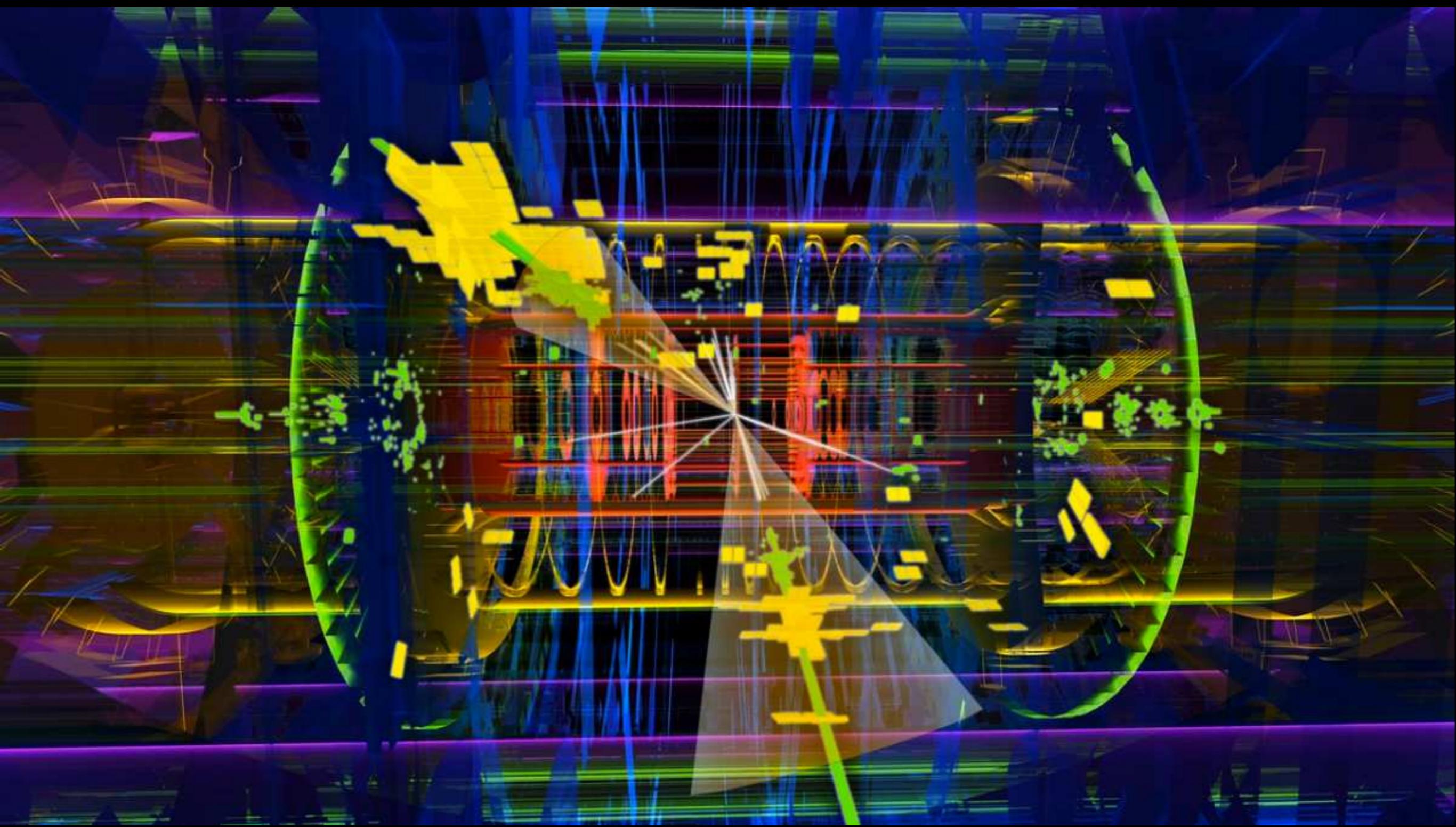
Crucial for physics at the Large Hadron Collider

- Mesons**
 $\pi^\pm \pi^0 \eta K^\pm K^0 \eta' D^\pm D^0 D_s^\pm \eta_c B^\pm B^0 B_s^0 \eta_b \dots$
 $\rho^\pm \rho^0 \omega K^{*\pm} K^{*0} \phi D^{*\pm} D^{*0} D_s^{*\pm} J/\psi B^{*\pm} B^{*0} B_s^{*0} \Upsilon \dots$
- Baryons**
 $p n \Lambda^0 \Sigma^+ \Sigma^0 \Sigma^- \Xi^0 \Xi^- \dots$
 $\Delta^{++} \Delta^+ \Delta^0 \Delta^- \Sigma^{*+} \Sigma^{*0} \Sigma^{*-} \Xi^{*0} \Xi^{*-} \Omega^- \dots$
- Tetraquarks**
 $X(3872) Y(4260) Z(4430) \dots$
- Pentaquarks**
 $P_c^+(4450) \dots$

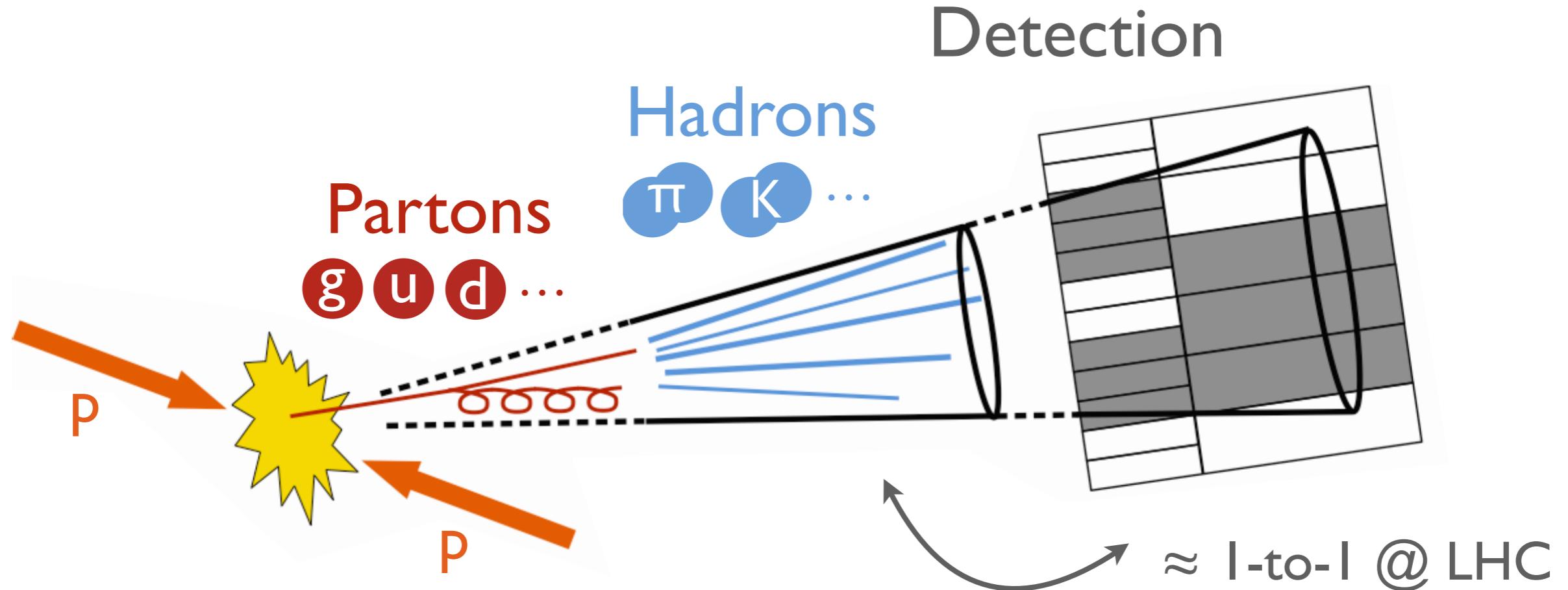




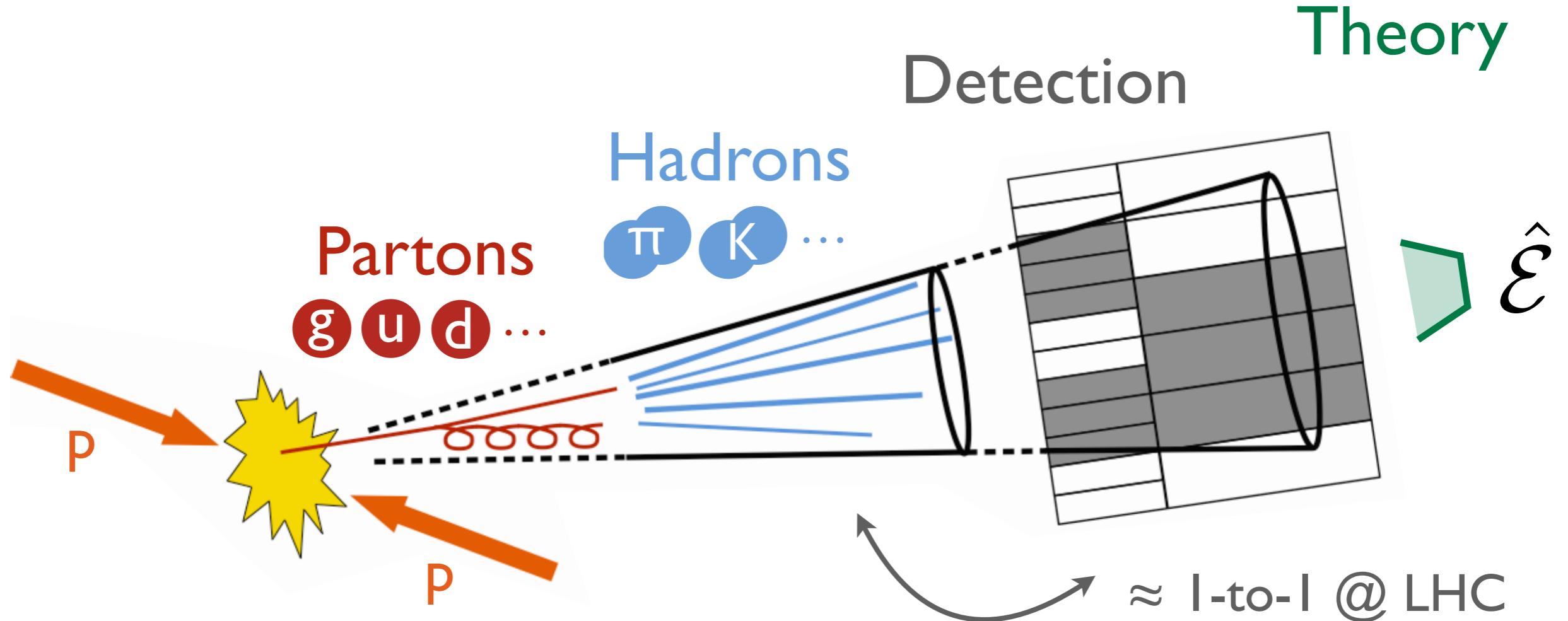




Jet Formation



Jet Formation

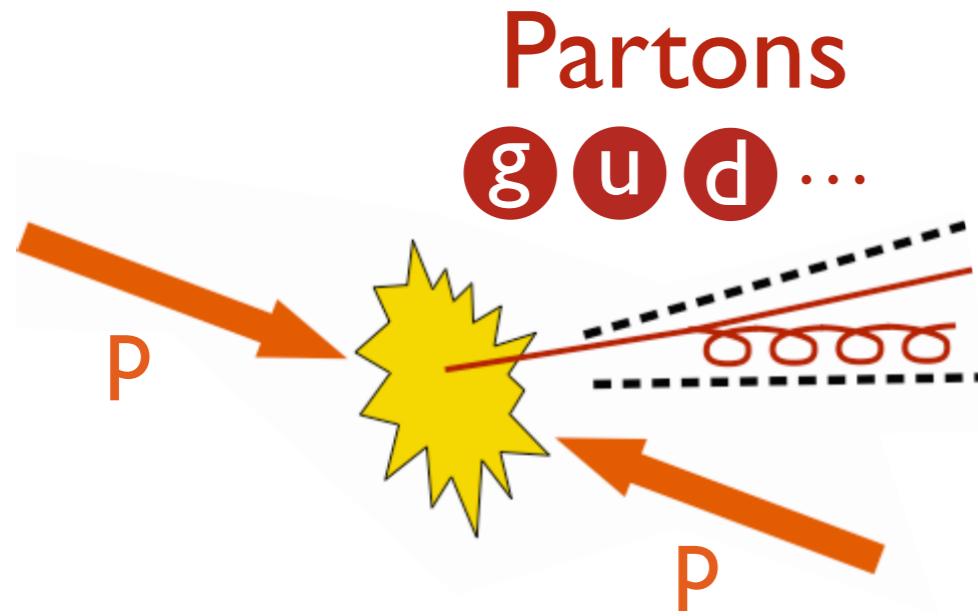


Physics described by **stress-energy flow**

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

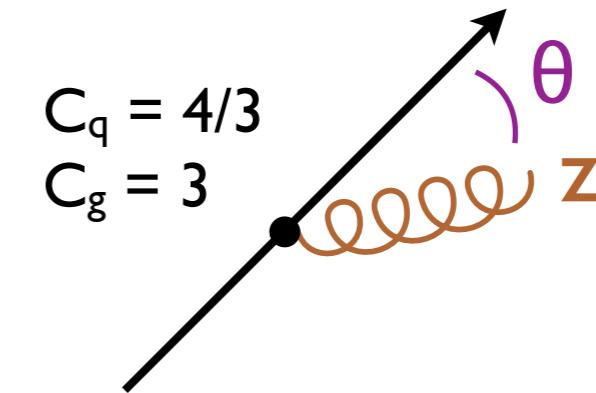
[Sveshnikov, Tkachov, [hep-ph/9512370](#); Hofman, Maldacena, [0803.1467](#); Mateu, Stewart, JDT, [1209.3781](#)]

Jet Formation



Altarelli-Parisi Splitting

Core prediction of QCD

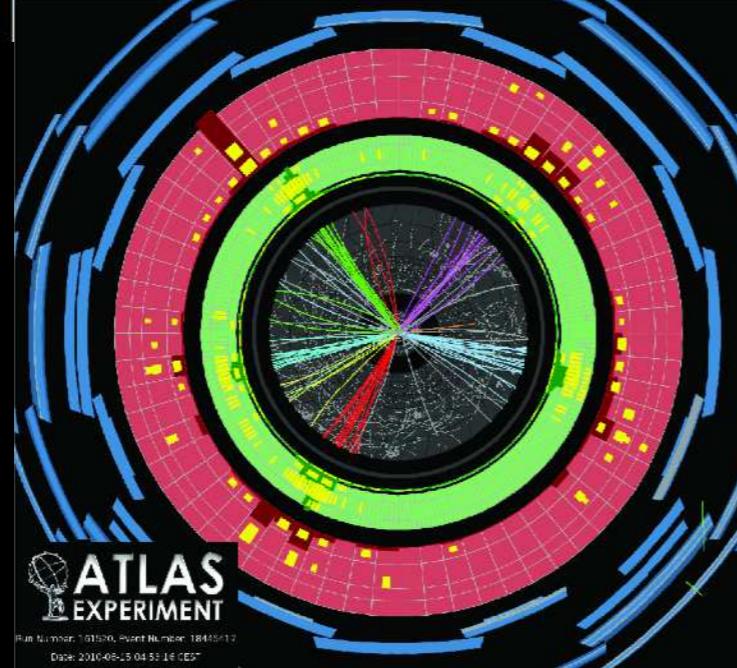
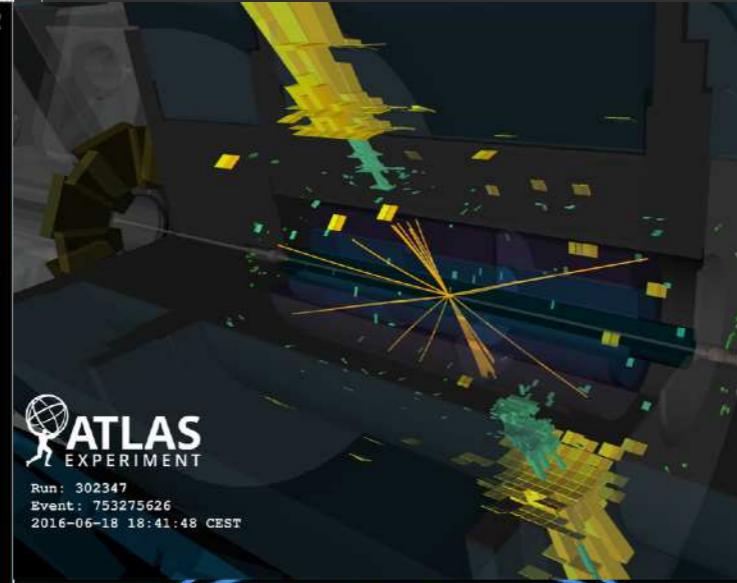
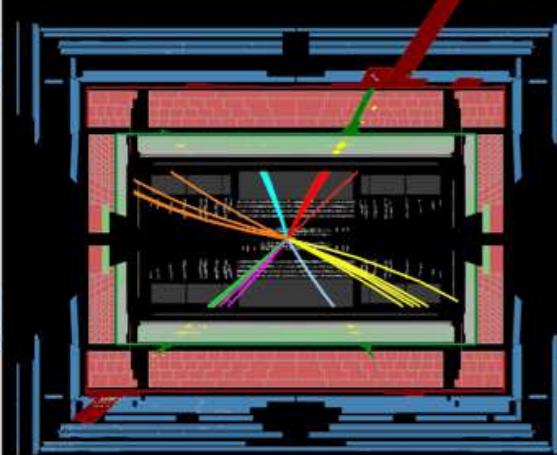


$$dP_{i \rightarrow ig} \simeq \frac{2\alpha_s}{\pi} C_i \frac{d\theta}{\theta} \frac{dz}{z}$$

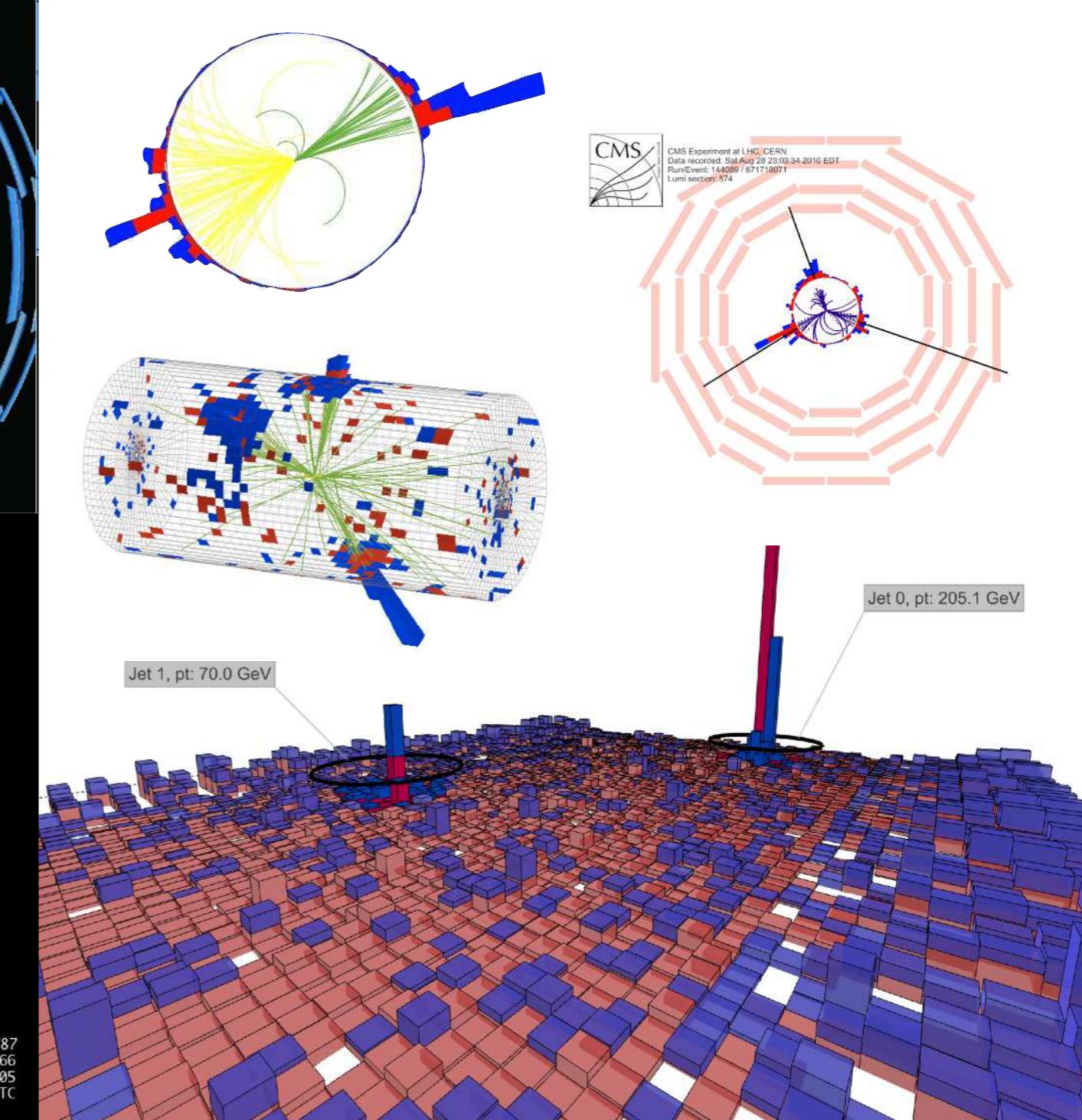
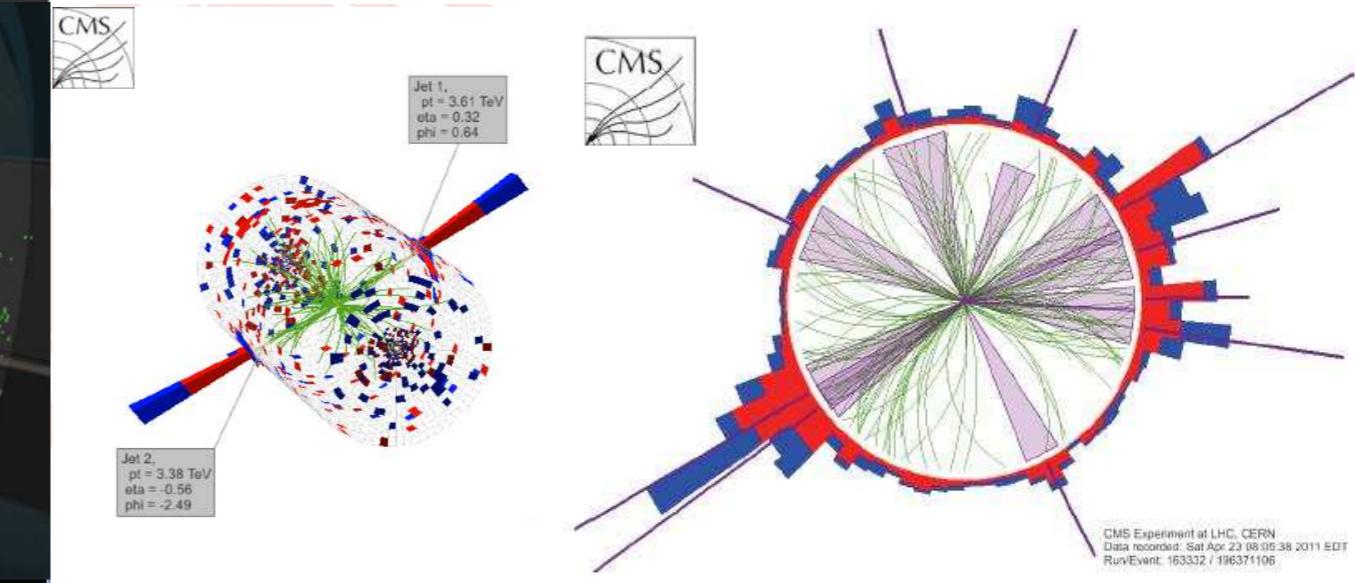
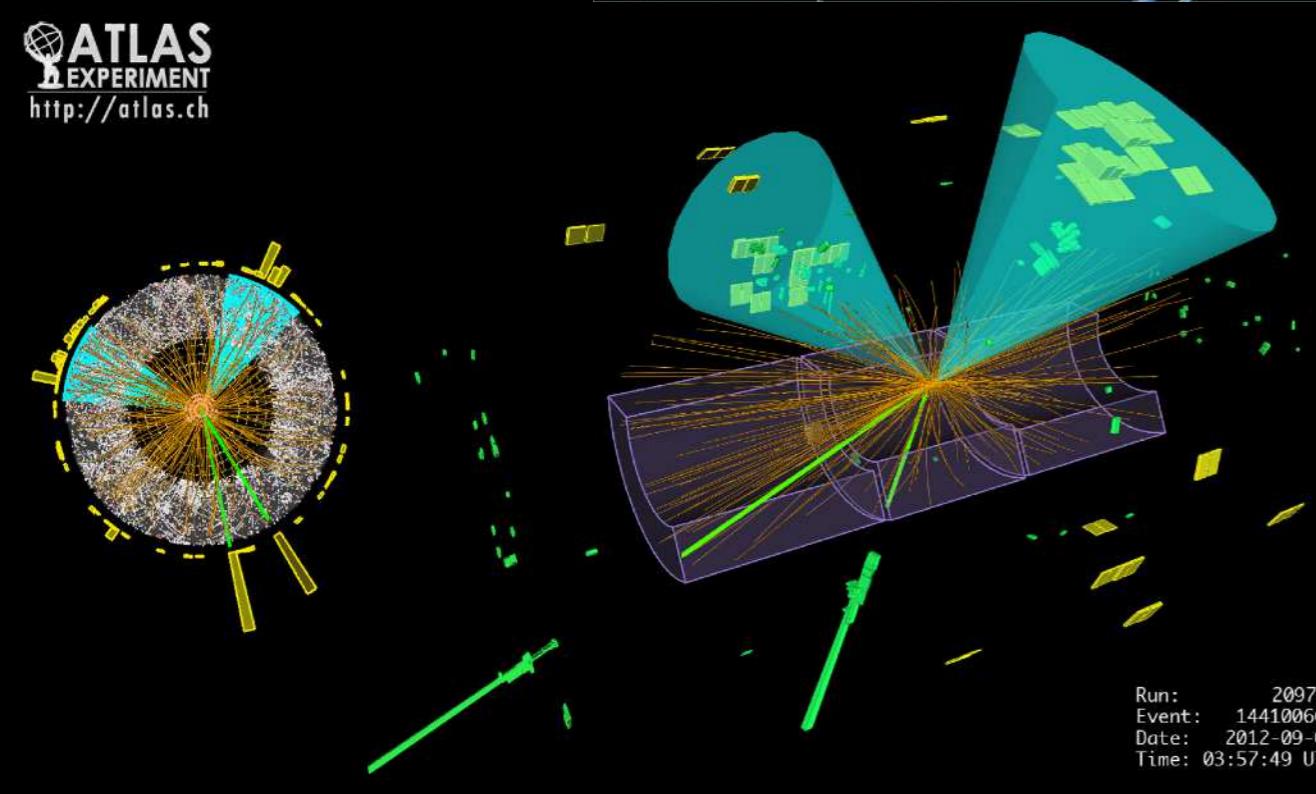
— Collinear — Soft

Run Number: 159224, Event Number: 3533152

Date: 2010-07-18 11:05:54 CEST

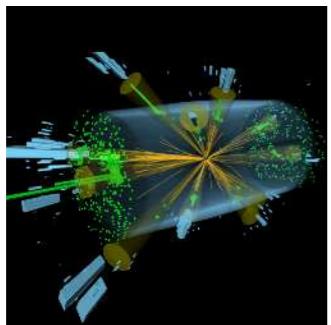


ATLAS
EXPERIMENT
<http://atlas.ch>

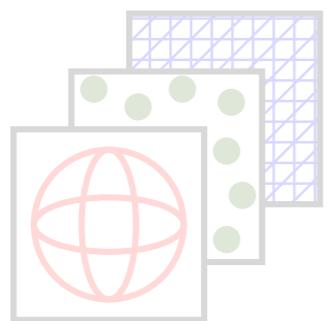




Particle Physics Primer

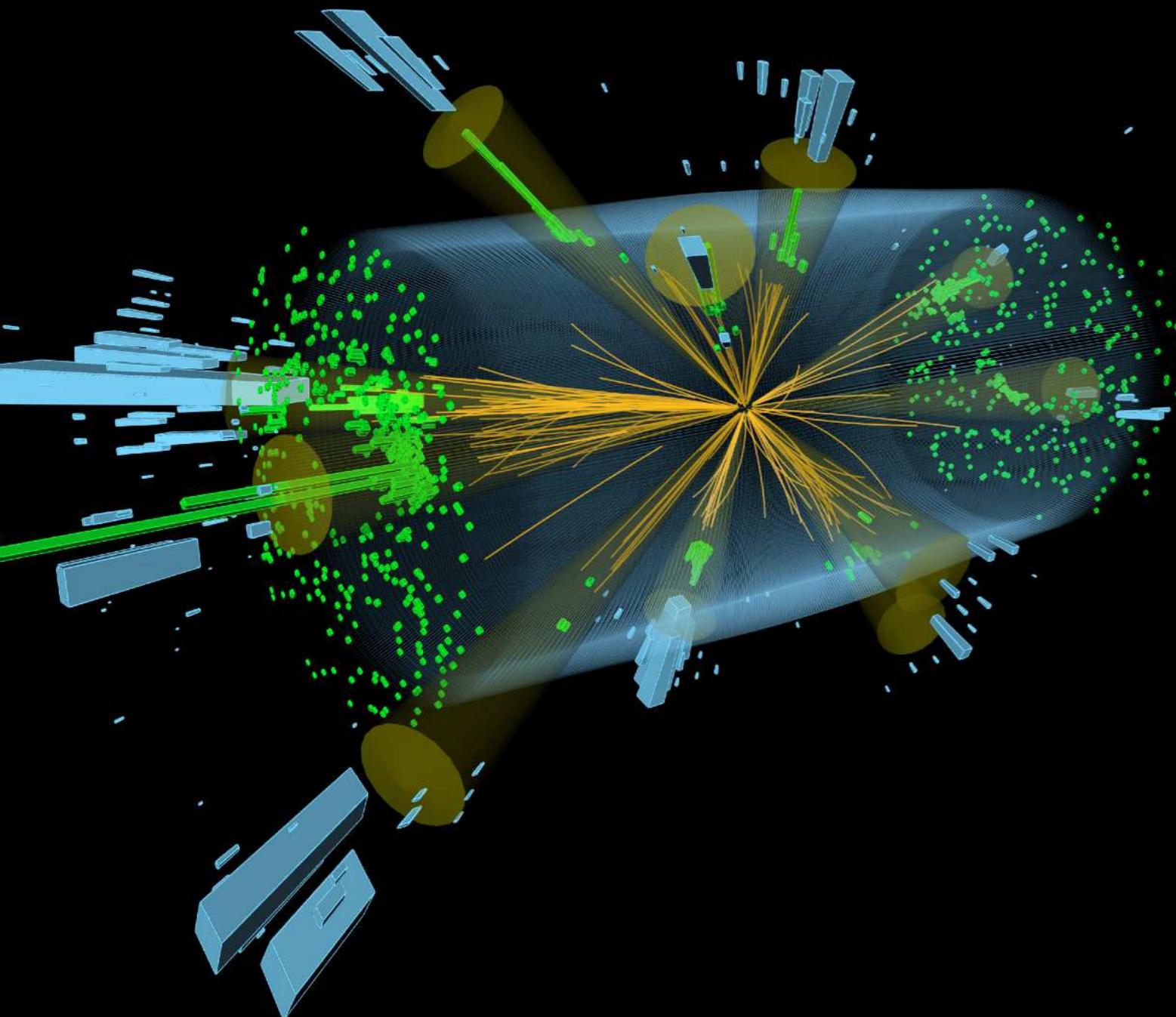


Jets and Point Clouds



Energy Flow Networks

What is a Collision Event?



T E H M

 γ

photon

 e^+

electron

 μ^+

muon

 π^+

pion

 K^+

kaon

 K_L^0

K-long

 p/\bar{p}

proton

 n/\bar{n}

neutron

elementary

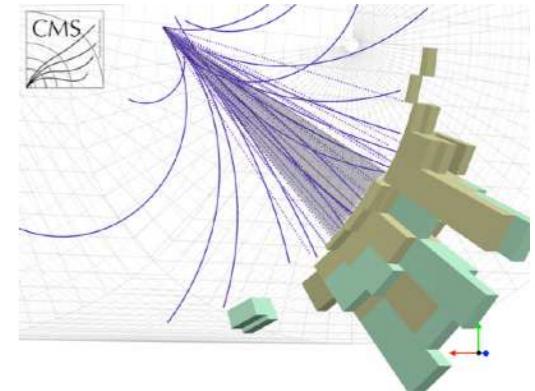
composite

Point Cloud



[Popular Science, 2013]

Key: Jets are Point Clouds



- **Particle:** List of properties

$$\vec{p} = \{E, p_x, p_y, p_z, \dots\}$$

↑ | ↑

Energy Momentum Mass, charge, flavor, vertex, quality, ...

- Jet: Set of particles

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



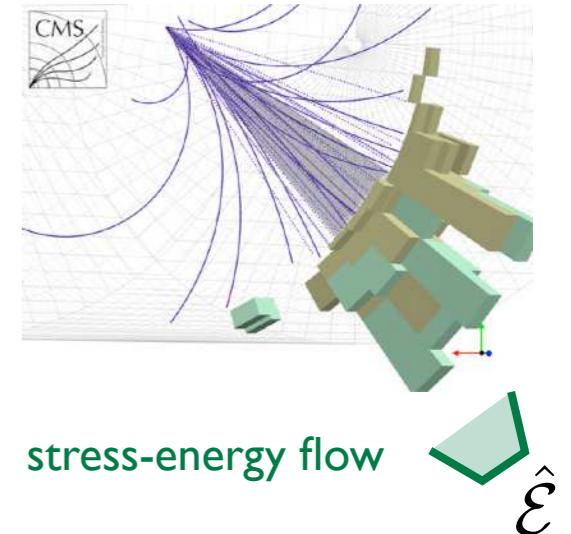
- Dataset: Set of jets

Optionally: Weighted Point Clouds

- Energy-weighted directions

$$\vec{p} = \{E, n_x, n_y, n_z\}$$

↑ ——————
Energy Direction



- Energy Flow: Set of energy-weighted directions

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

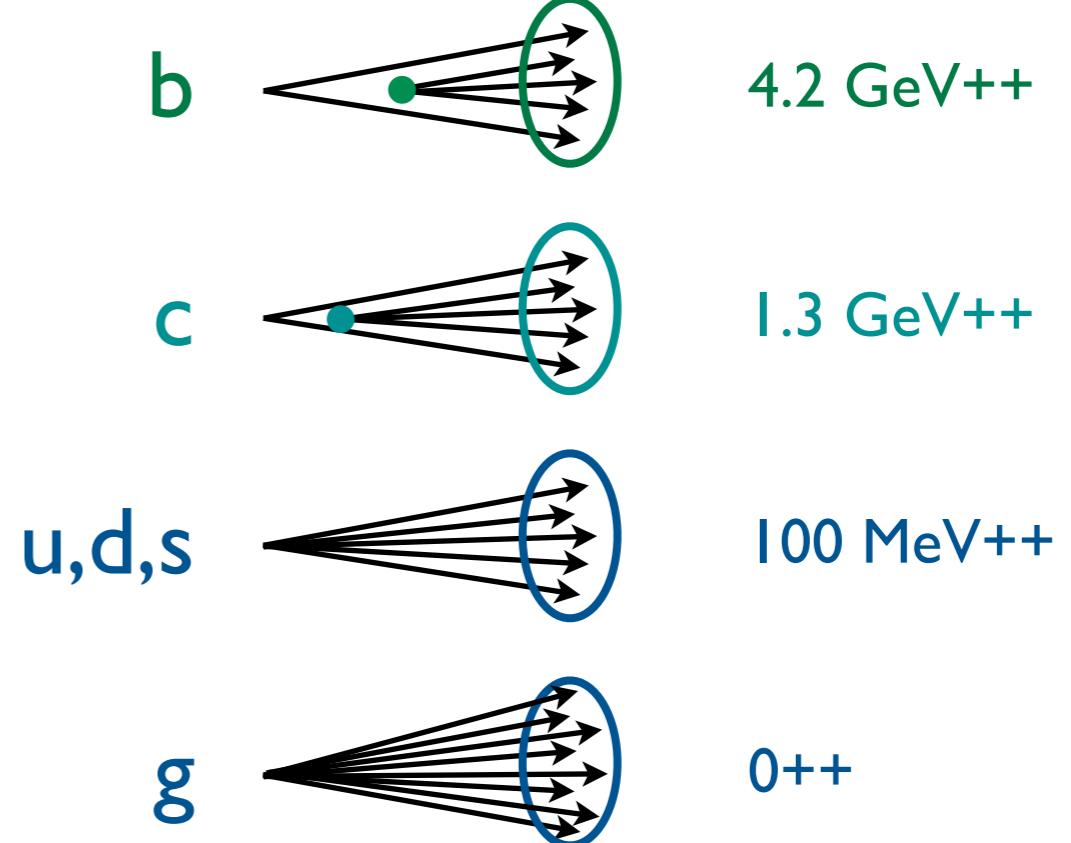
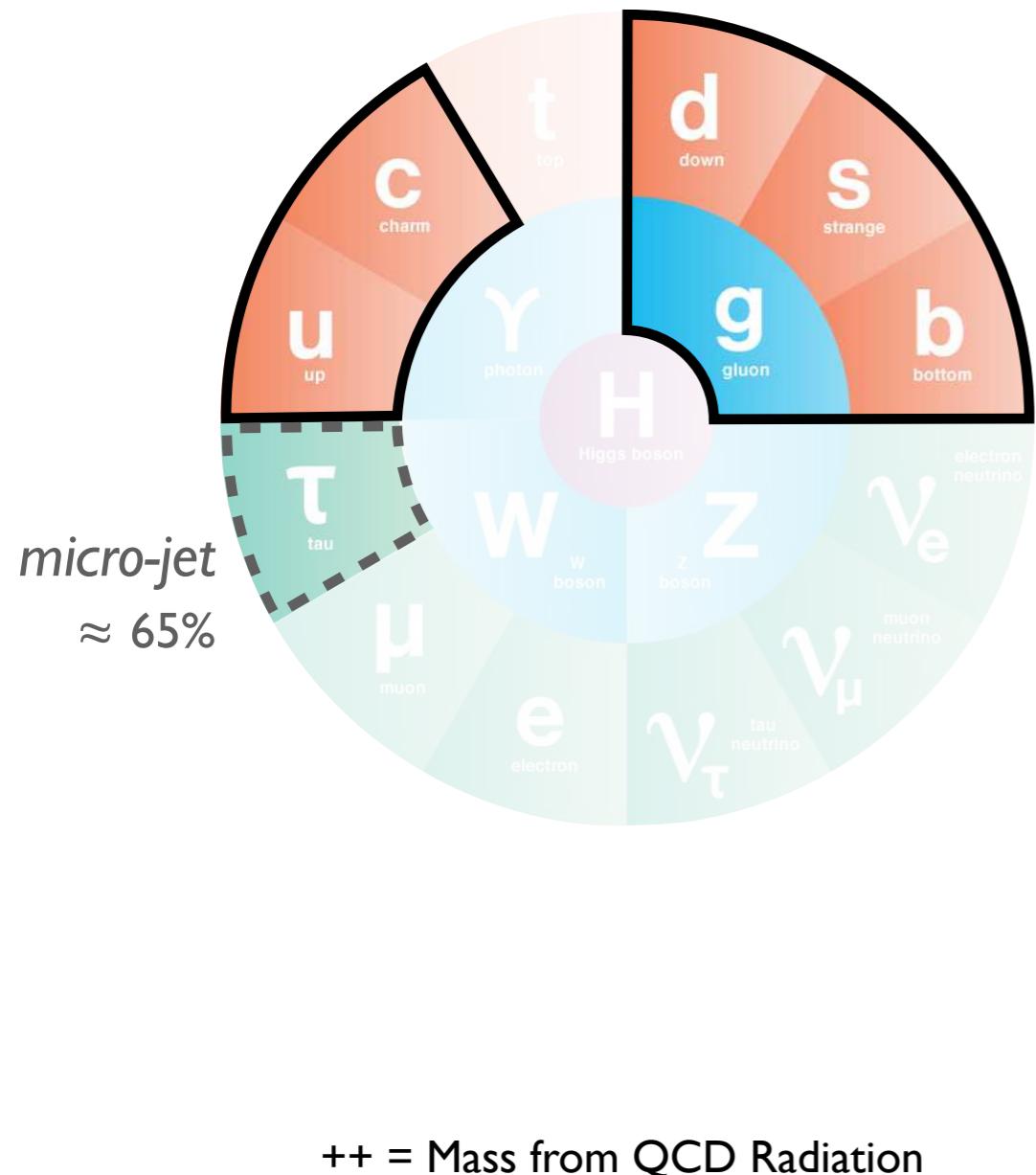
- “Safe” to Altarelli-Parisi splitting

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



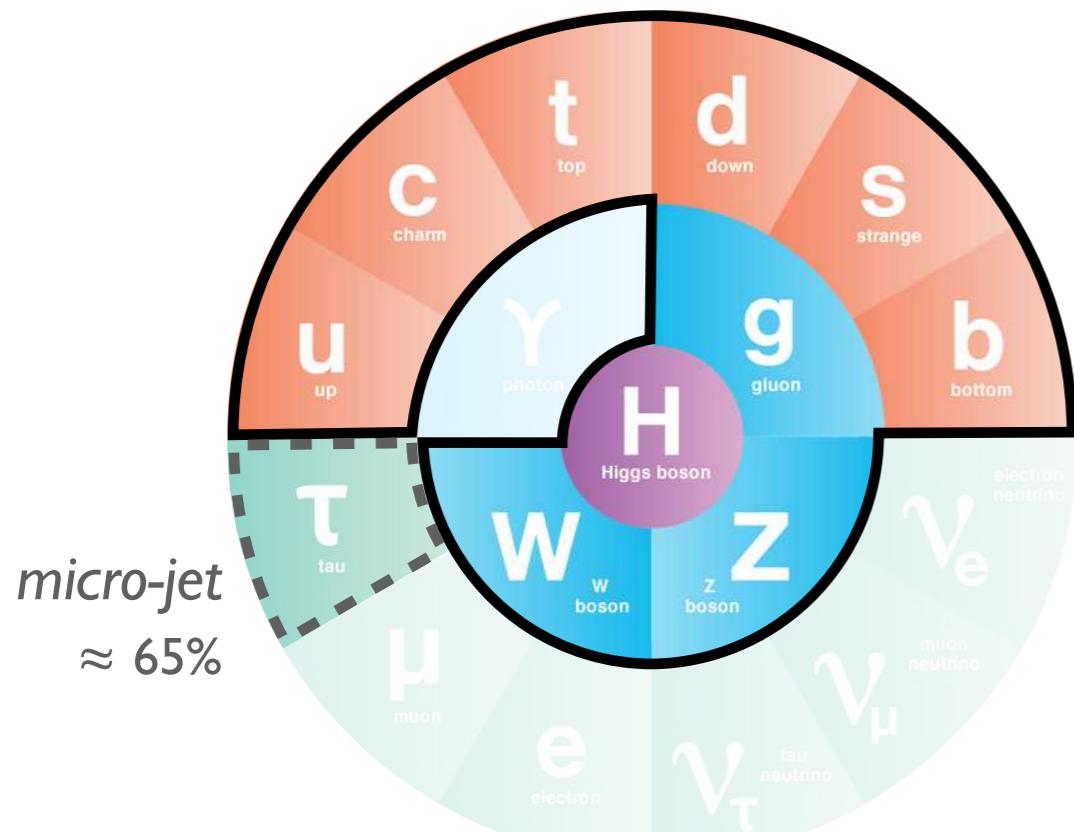
Jet Classification

One of many important LHC tasks

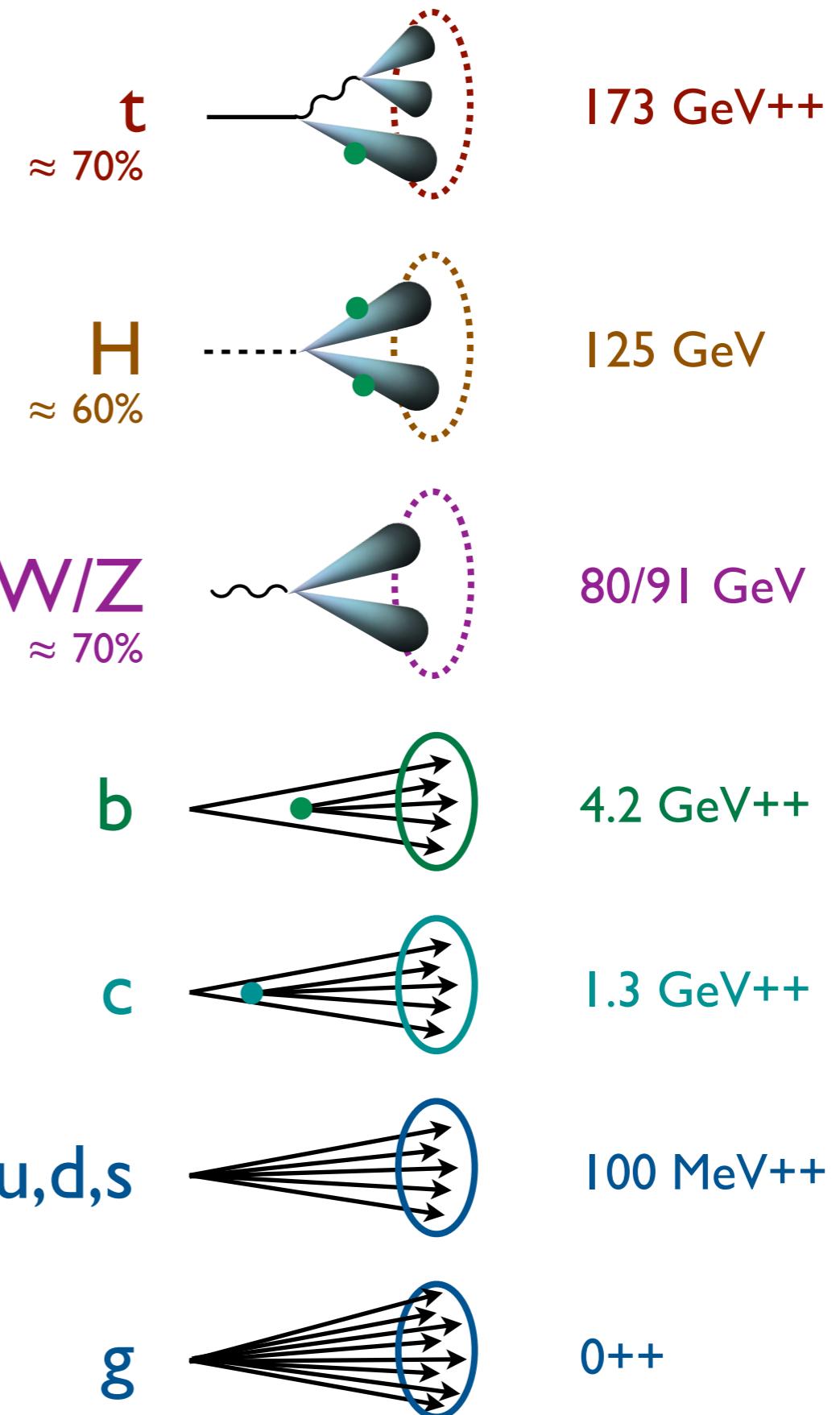


Jet Classification

One of many important LHC tasks

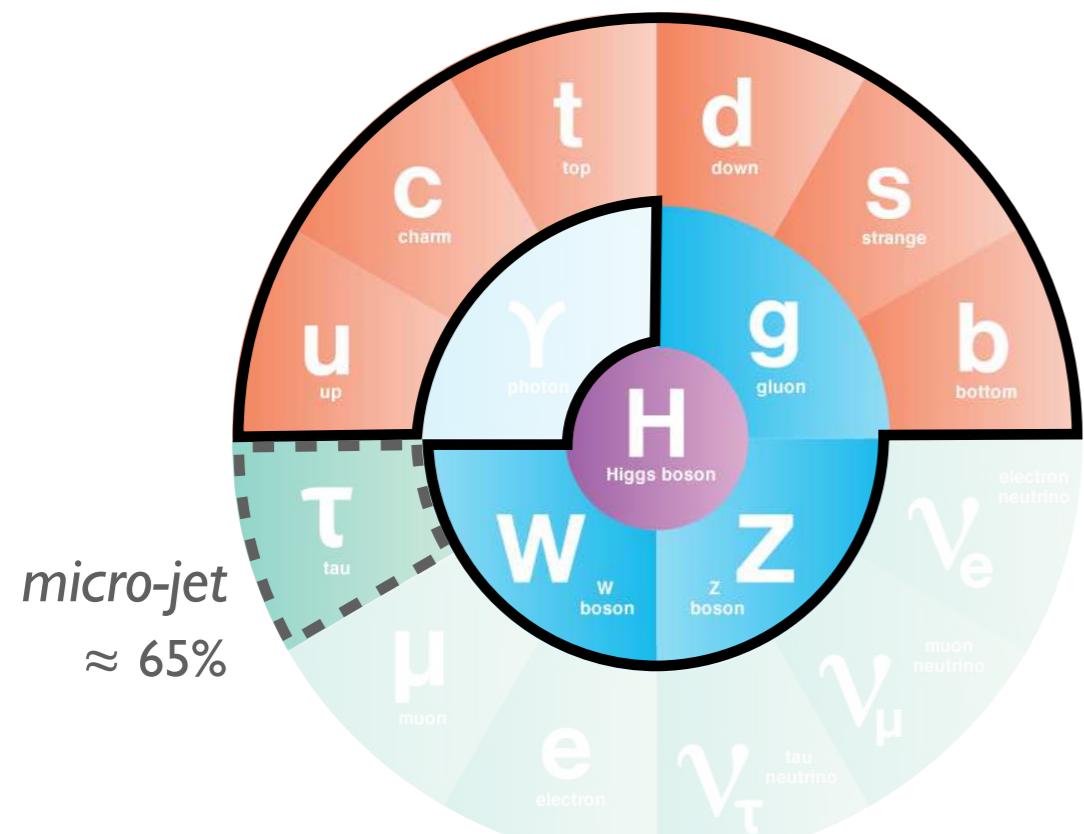


++ = Mass from QCD Radiation

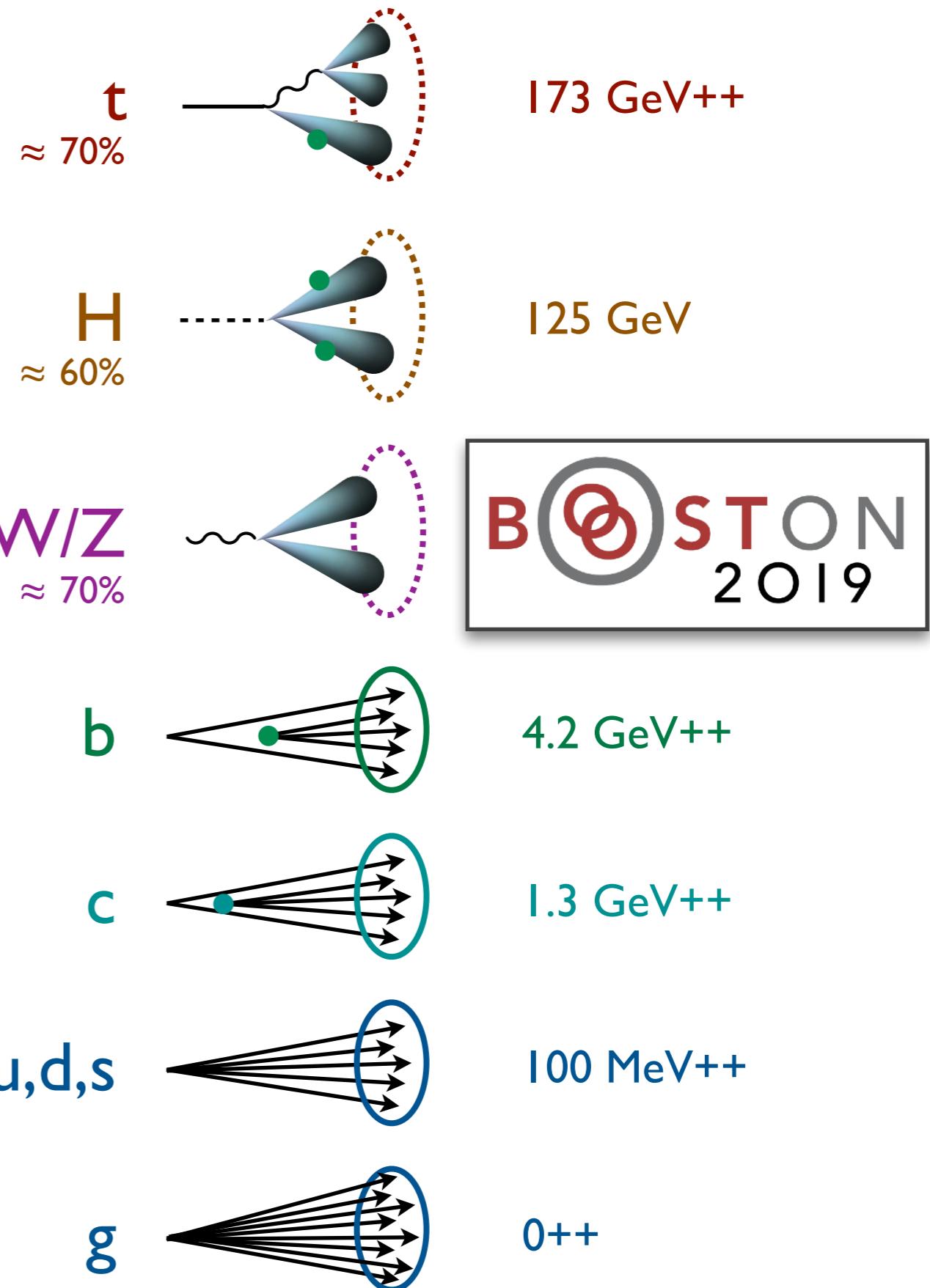


Jet Classification

One of many important LHC tasks

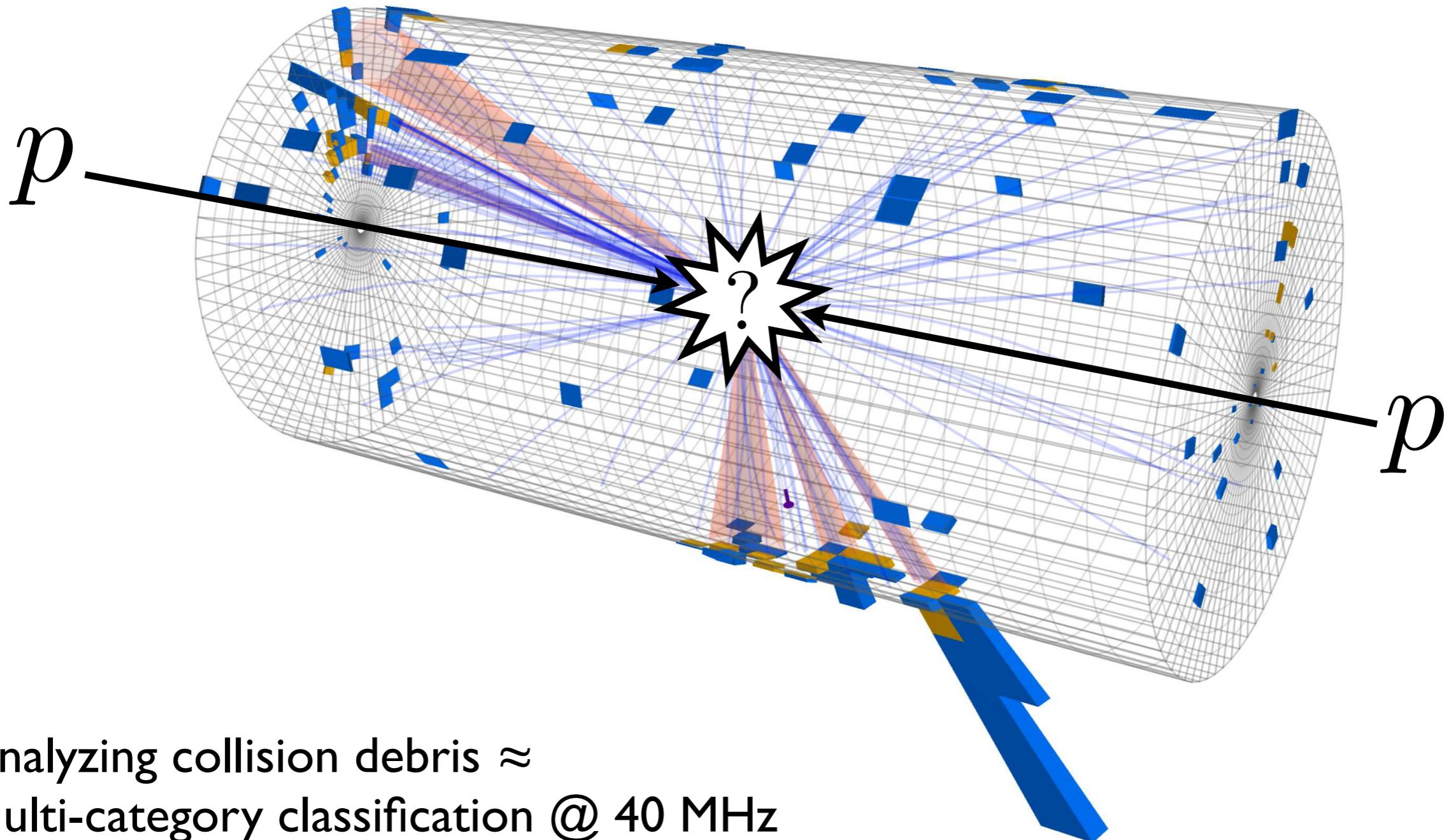


++ = Mass from QCD Radiation





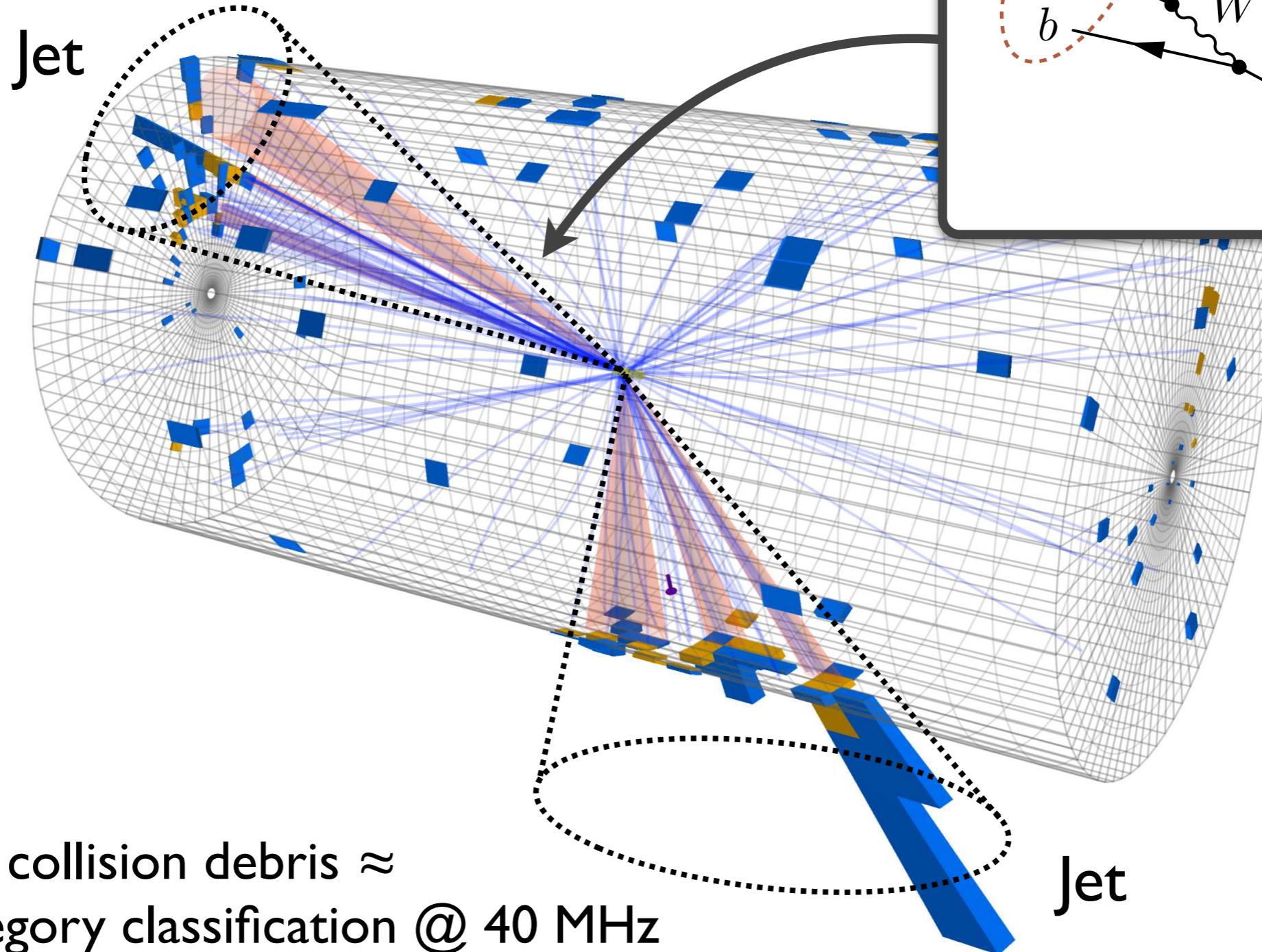
CMS Experiment at LHC, CERN
Data recorded: Sun Jul 12 07:25:11 2015 CEST
Run/Event: 251562 / 111132974
Lumi section: 122
Orbit/Crossing: 31722792 / 2253



Analyzing collision debris ≈
Multi-category classification @ 40 MHz



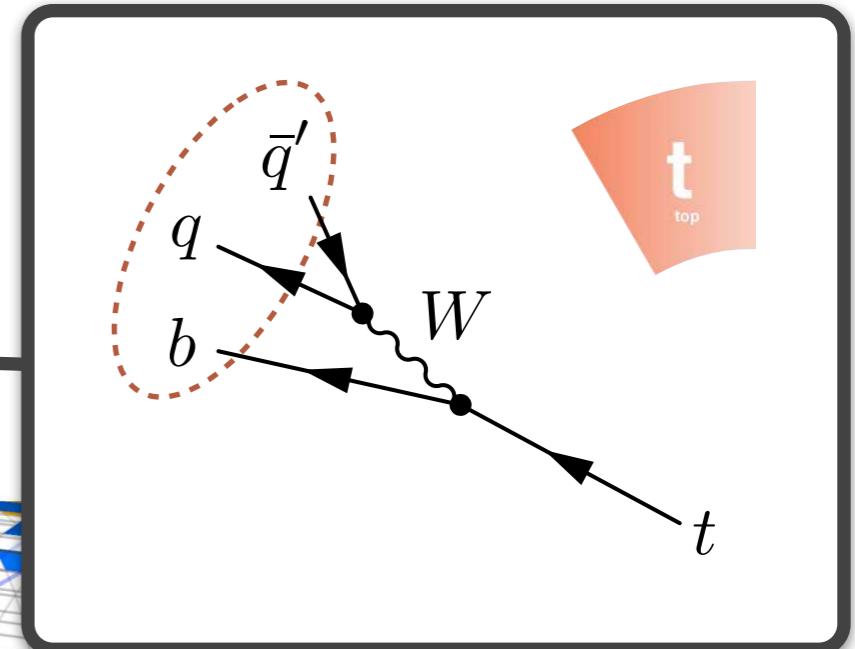
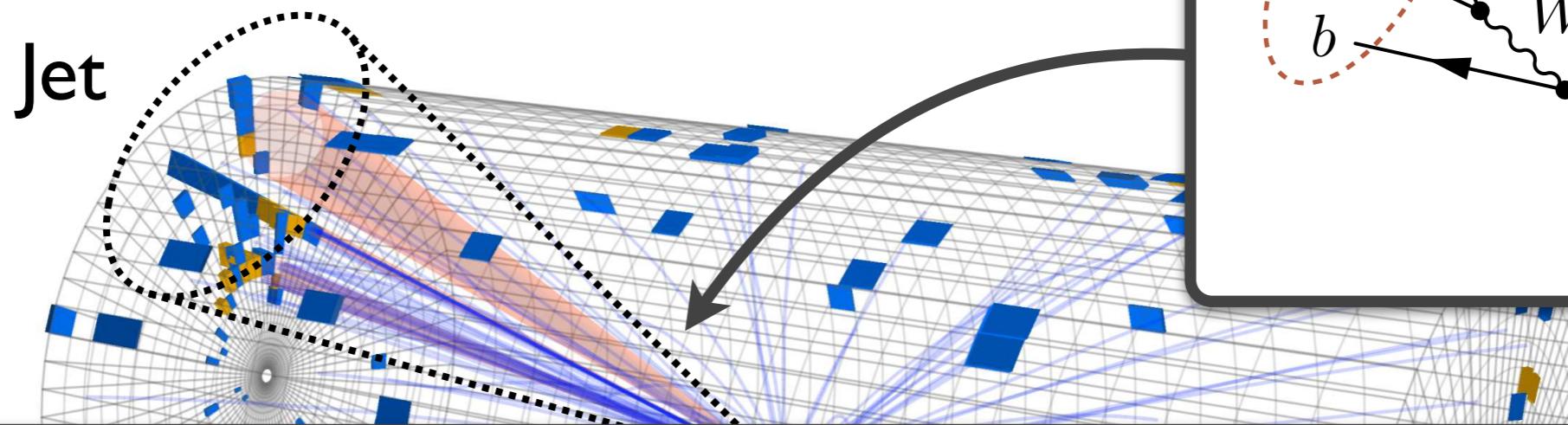
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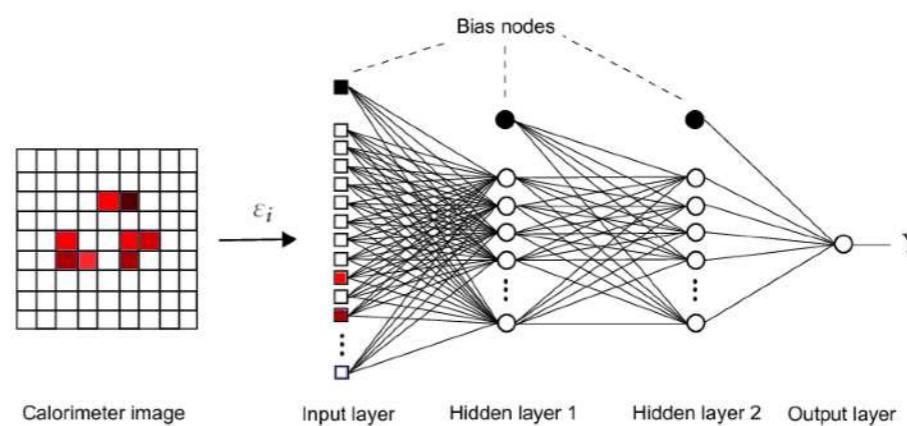
“Deep Thinking”?

[e.g. JDT, Van Tilburg, [1011.2268](#), [1108.2701](#);
 rephrased in language of Komiske, Metodiev, JDT, [1902.02346](#)]

$$\tau_N(\mathcal{J}) = \min_{|\mathcal{J}'|=N} \text{EMD}(\mathcal{J}, \mathcal{J}')$$

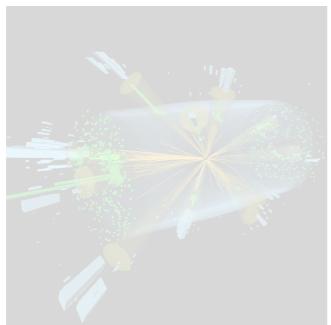
“Deep Learning”?

[e.g. Almeida, Backović, Cliche, Lee, Perelstein, [1501.05968](#);
 review in Kasieczka, Plehn, et al. (Komiske, Metodiev), [1902.09914](#)]

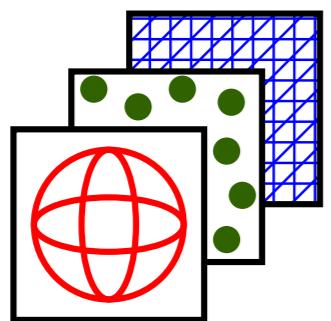




Particle Physics Primer



Jets and Point Clouds



Energy Flow Networks

Today's Goal

Teach a Machine to Communicate to a Physicist

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

Unordered, Variable Length Set

Safety: $\vec{p} = \{ E, n_x, n_y, n_z \}$

(optional)

Energy weighting

Properly specified
problem



The
Machine

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



Solution

$S(\mathcal{J})$

Verification

$V(\mathcal{J})$

(Theoretical)
Particle
Physics



Patrick Komiske



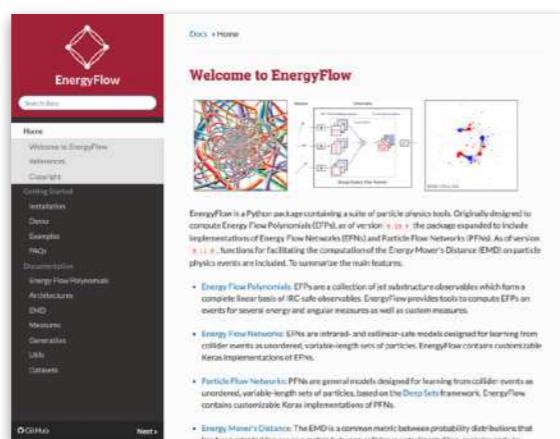
Eric Metodiev



Thank you!



Mathematics,
Statistics,
Computer Science



Energy Flow Networks

<https://energyflow.network/>

Building the Verification Function

Addition: Starting point for most “Deep Thinking”

$$\text{Additive Verification: } V(\mathcal{J}) = \sum_{i \in \mathcal{J}} \Phi(\vec{p}_i)$$

↓
Permutation symmetry
↑
Per particle function

$$\text{Safe Additive Verification: } V(\mathcal{J}) = \sum_{i \in \mathcal{J}} E_i \Phi(\vec{n}_i)$$

↑
Energy weighting ↑
 Per direction function

Building the Solution Function

“Deep Learning” based on Additive Verification?

Solution:

Interpretable Latent Space

$$S(\mathcal{J}) = F(V_1, V_2, \dots, V_\ell)$$
$$V_a(\mathcal{J}) = \sum_{i \in \mathcal{J}} \Phi_a(\vec{p}_i)$$

Parametrized with Neutral Networks

The diagram illustrates the solution function $S(\mathcal{J})$ as a function of V_1, V_2, \dots, V_ℓ . These latent variables V_i are shown as inputs to a function F . Above the equation, the text "Interpretable Latent Space" is written in purple. Below the equation, the text "Parametrized with Neutral Networks" is written in orange. The V functions are shown as dashed boxes with arrows pointing from \mathcal{J} to them, and another arrow points from each V function to the F function. The V functions are also labeled with a subscript a , indicating they are specific to a particular component a .

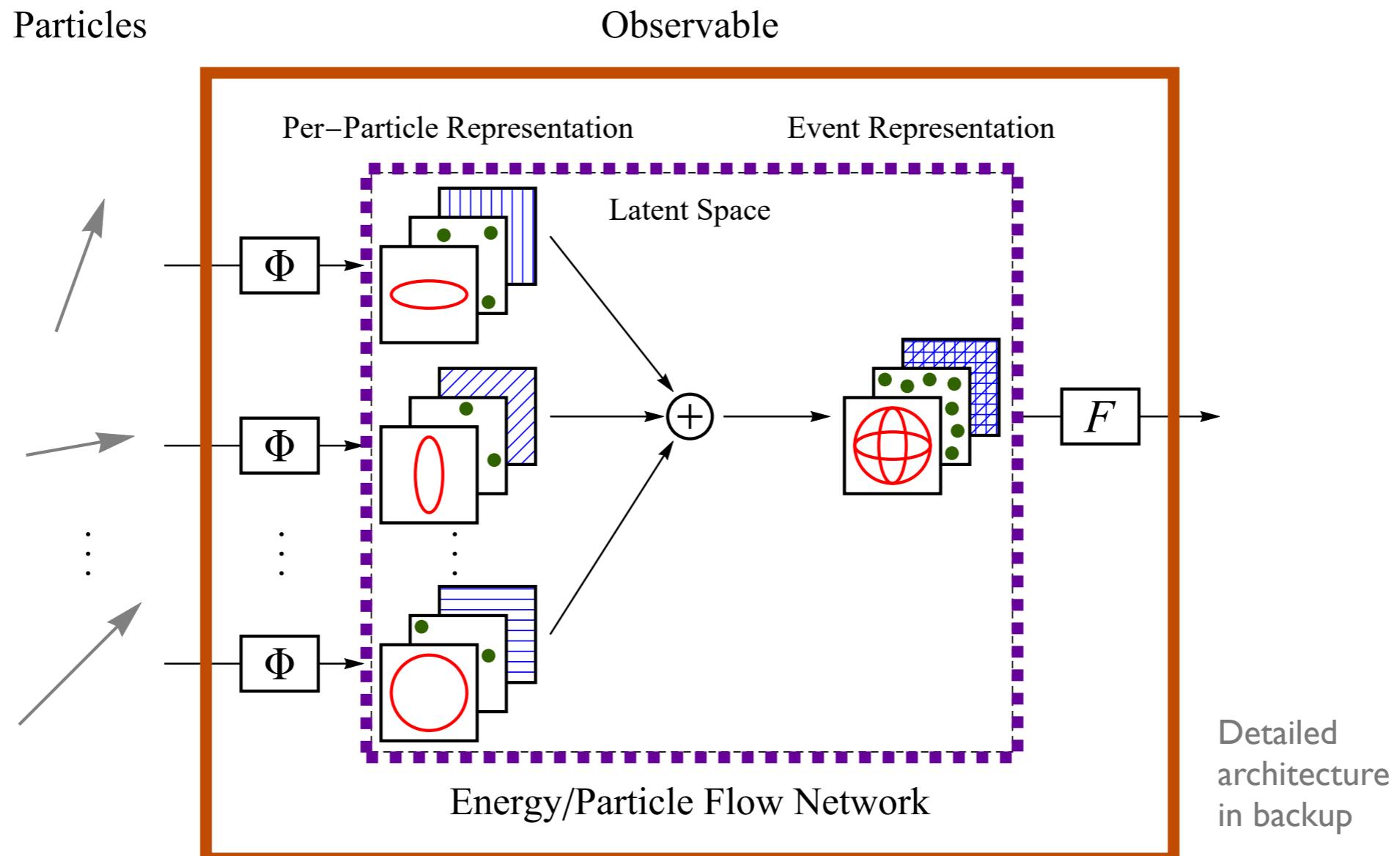
Energy / Particle Flow Networks

Safe Φ

General Φ

[Komiske, Metodiev, JDT, 1810.05165]

Whatever **solution** the network learns...

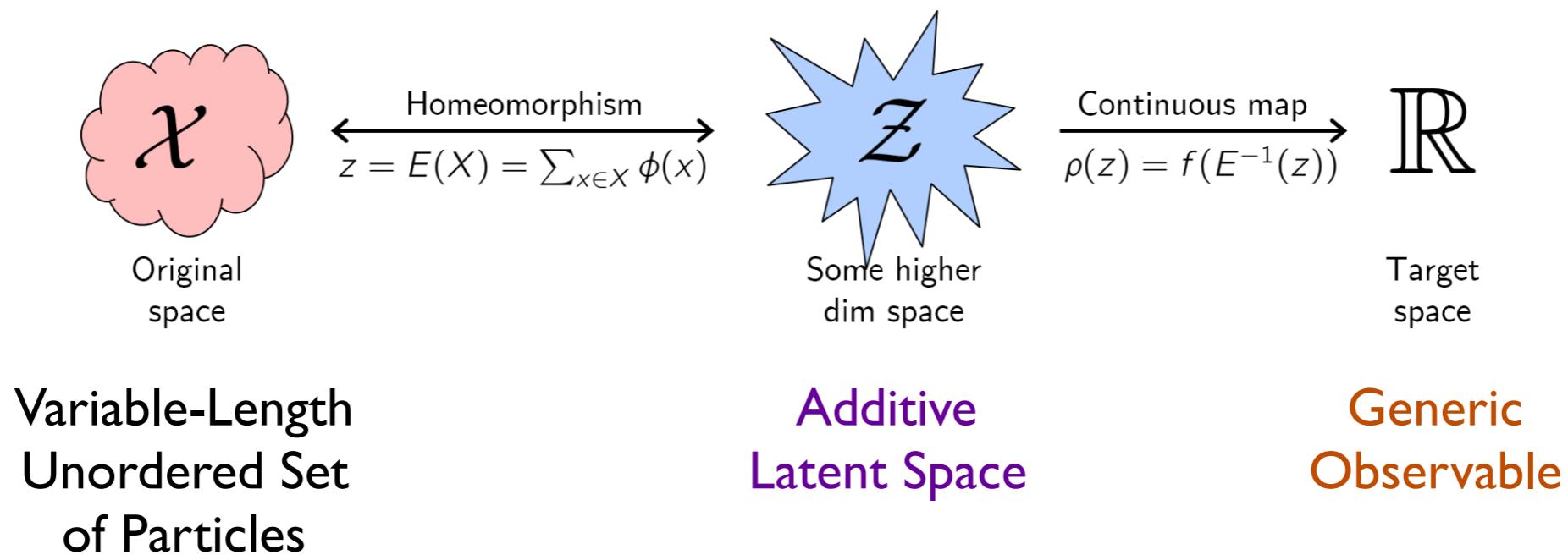


...we can **verify** the latent space

Meanwhile in ML-Land: Deep Sets

Theorem 2 A function $f(X)$ operating on a set X having elements from a countable universe, is a valid set function, i.e., **invariant** to the permutation of instances in X , iff it can be decomposed in the form $\rho(\sum_{x \in X} \phi(x))$, for suitable transformations ϕ and ρ .

↑
(!)



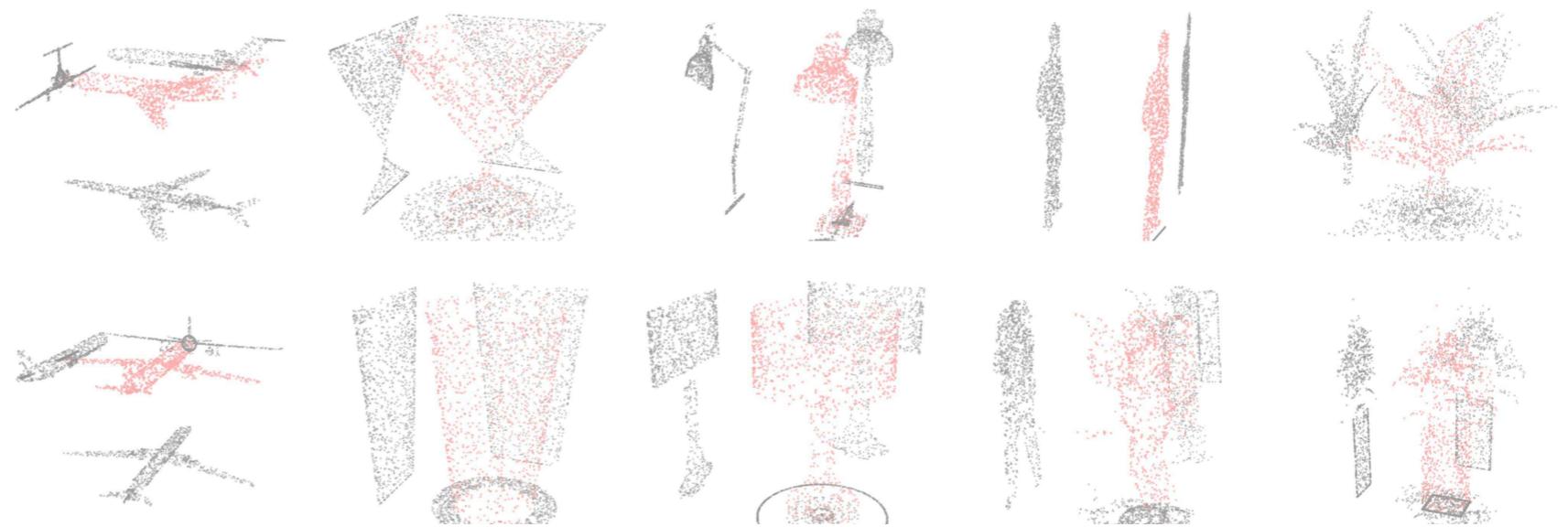
[Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, [1703.06114](#); see also Vinyals, Bengio, Kudlur, [1511.06391](#); Qi, Su, Mo, Guibas, [1612.00593](#)]

Deep Sets for...

Celebrity Face Anomaly Detection

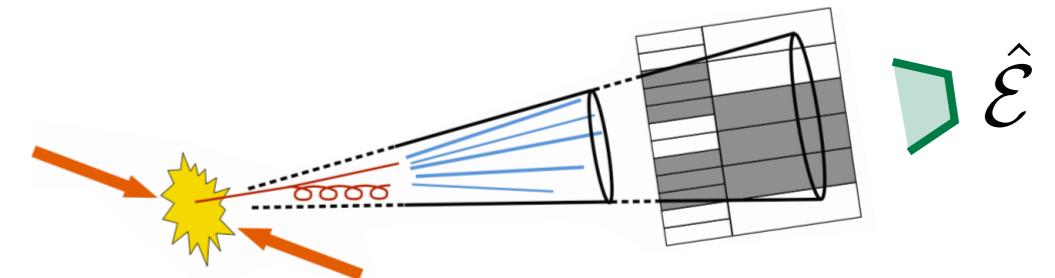
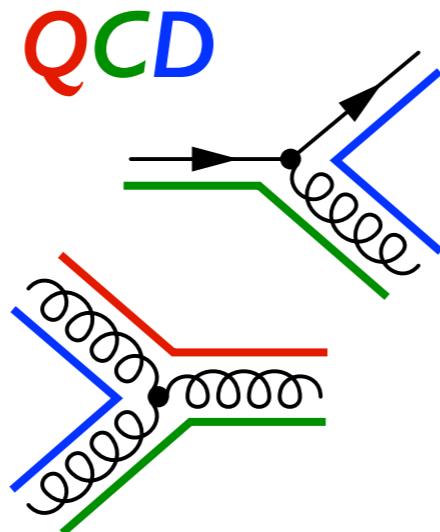
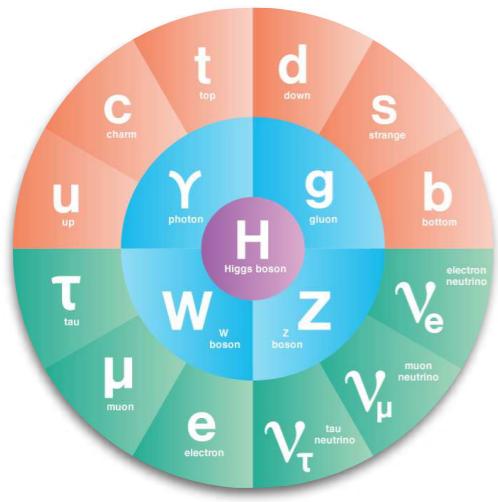


Point Cloud Classification

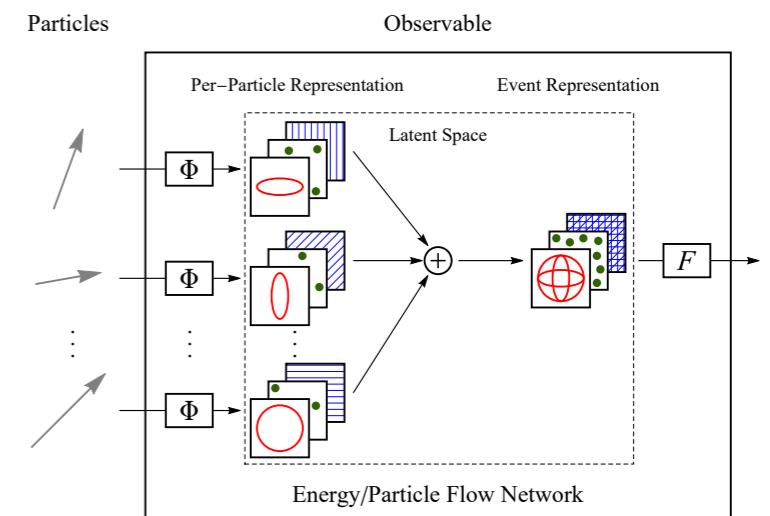
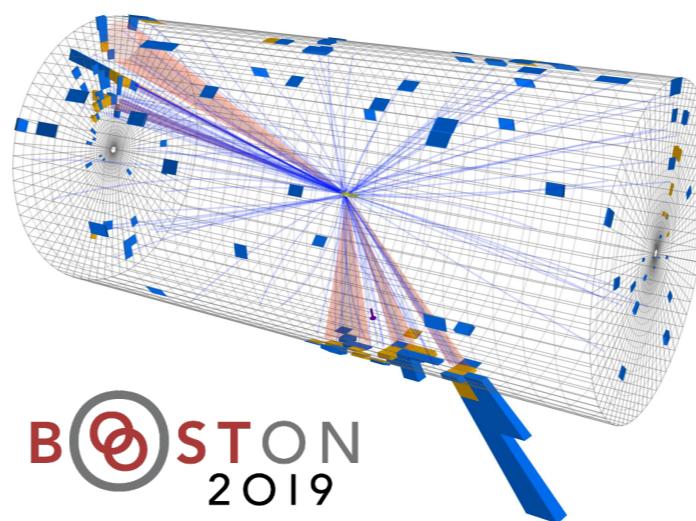
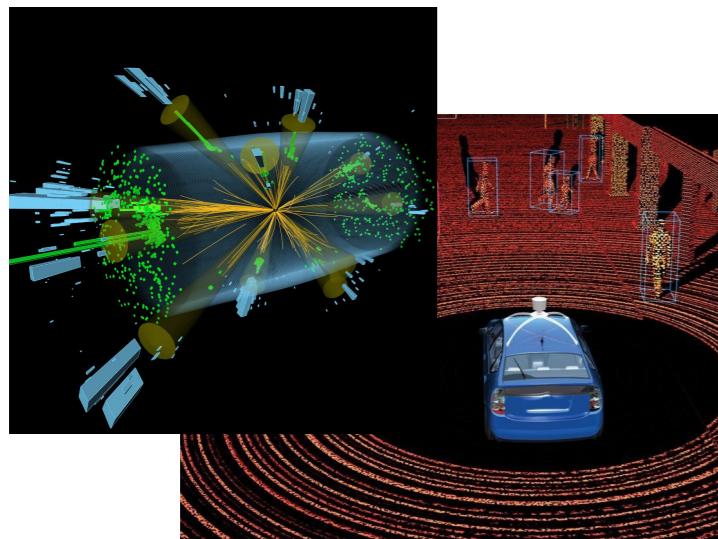


[Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, [1703.06114](#)]

Deep Sets for Particle Jets



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



Quark vs. Gluon

The “Hello, World!” of jet classification

1. Specify the problem
2. Find the solution
3. Verify the solution



Find $S\left(\begin{array}{c} \nearrow \\ \nearrow \\ \nearrow \end{array}\right)$ such that

$$S(\text{Quark}) = 1$$
$$S(\text{Gluon}) = 0$$

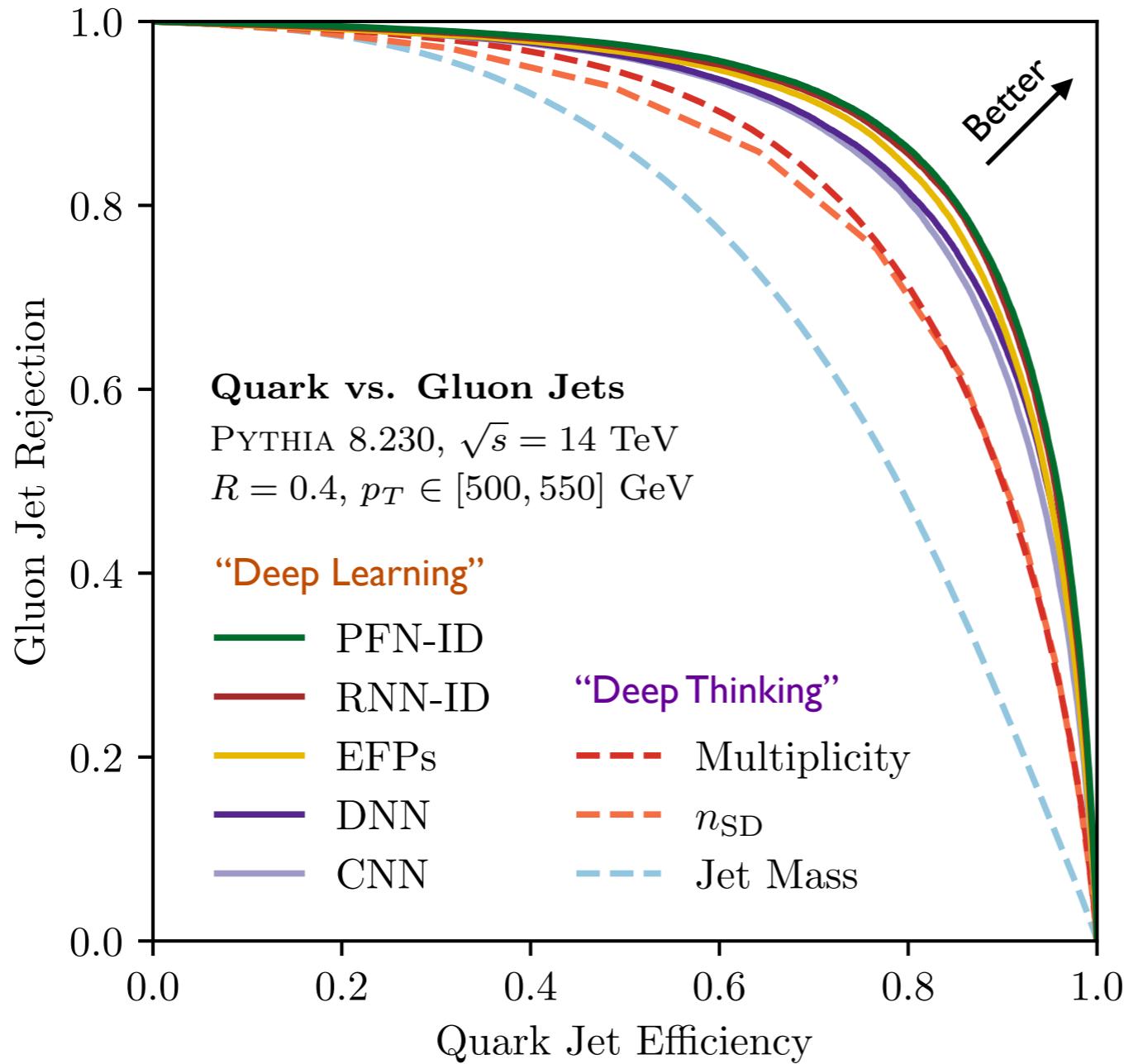
Best you can do: $S(\mathcal{J}) = \frac{p(\mathcal{J}|Q)}{p(\mathcal{J}|Q) + p(\mathcal{J}|G)}$

(Neyman-Pearson lemma)

Quark vs. Gluon

The “Hello, World!” of jet classification

1. Specify the problem
2. Find the solution
3. Verify the solution



*ML does
amazingly well*

[Komiske, Metodiev, JDT, 1810.05165]

Quark vs. Gluon

The “Hello, World!” of jet classification

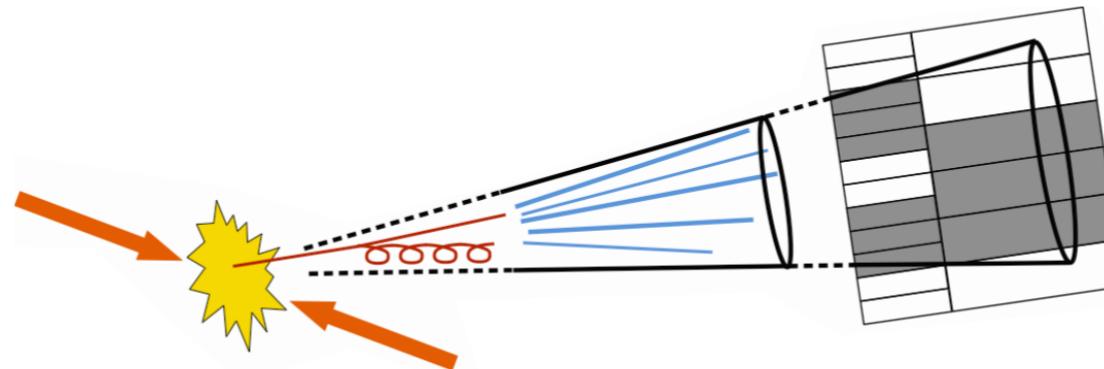
1. Specify the problem
2. Find the solution
3. Verify the solution

Energy Flow Networks: *ML designed to not get in the way*

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



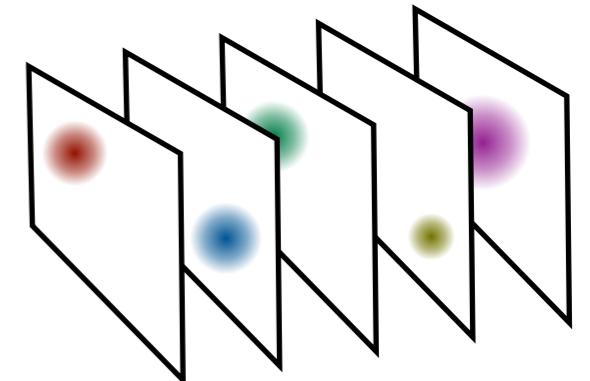
Difficult to visualize
(unless ℓ is small)



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



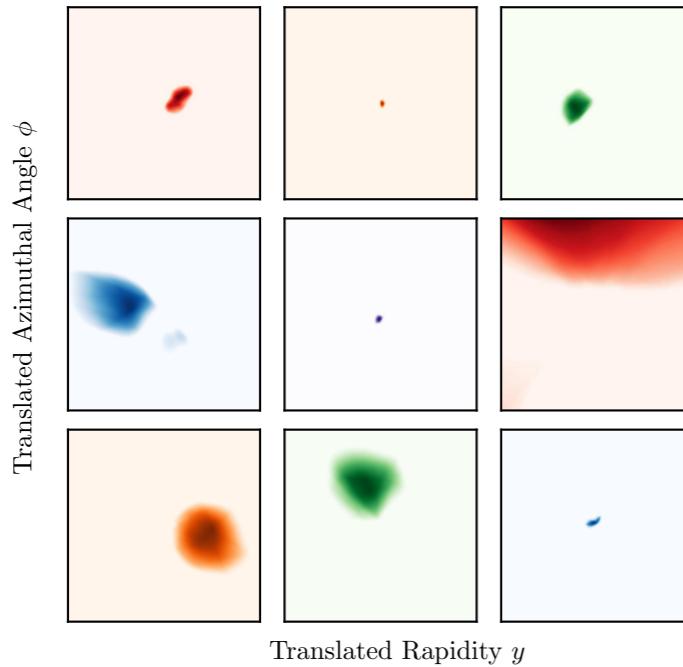
Easy to plot these!



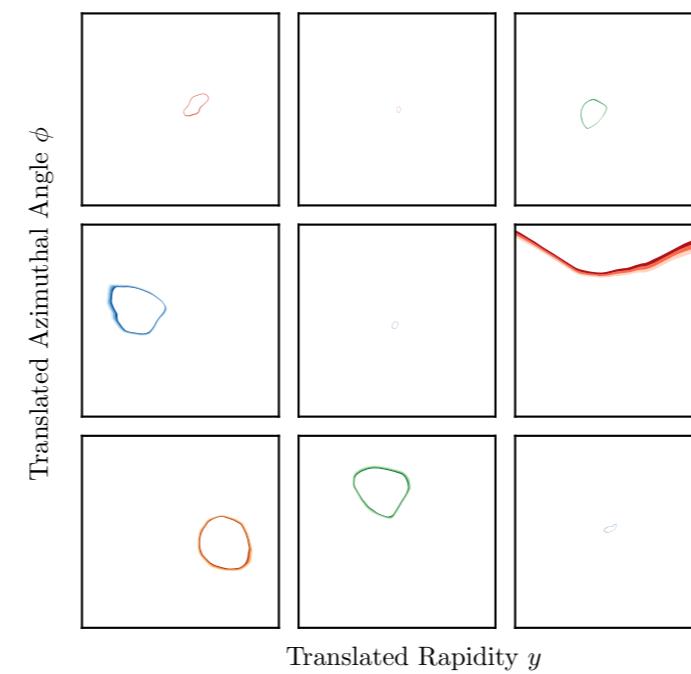
(similar to CNN filter activation)

Psychedelic Network Visualization

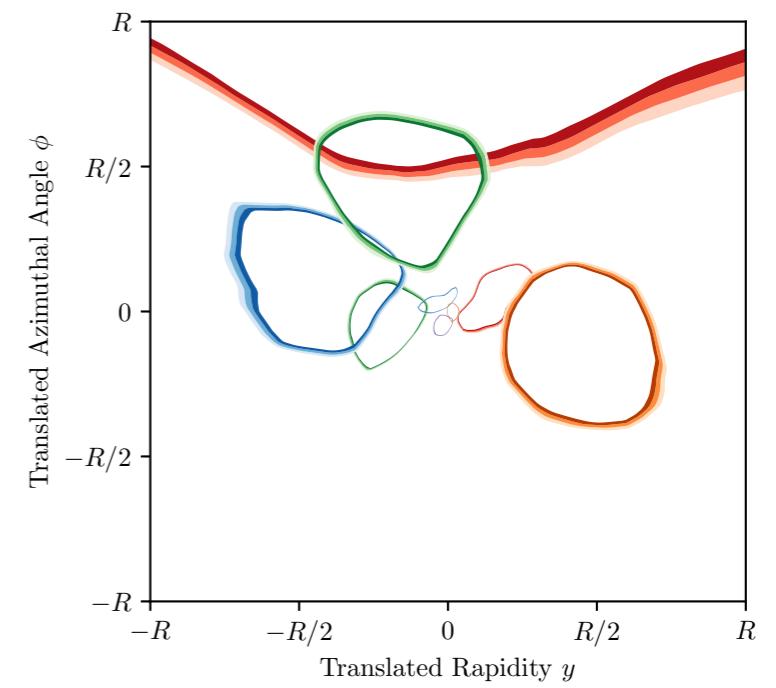
Latent Filters



50% Contours

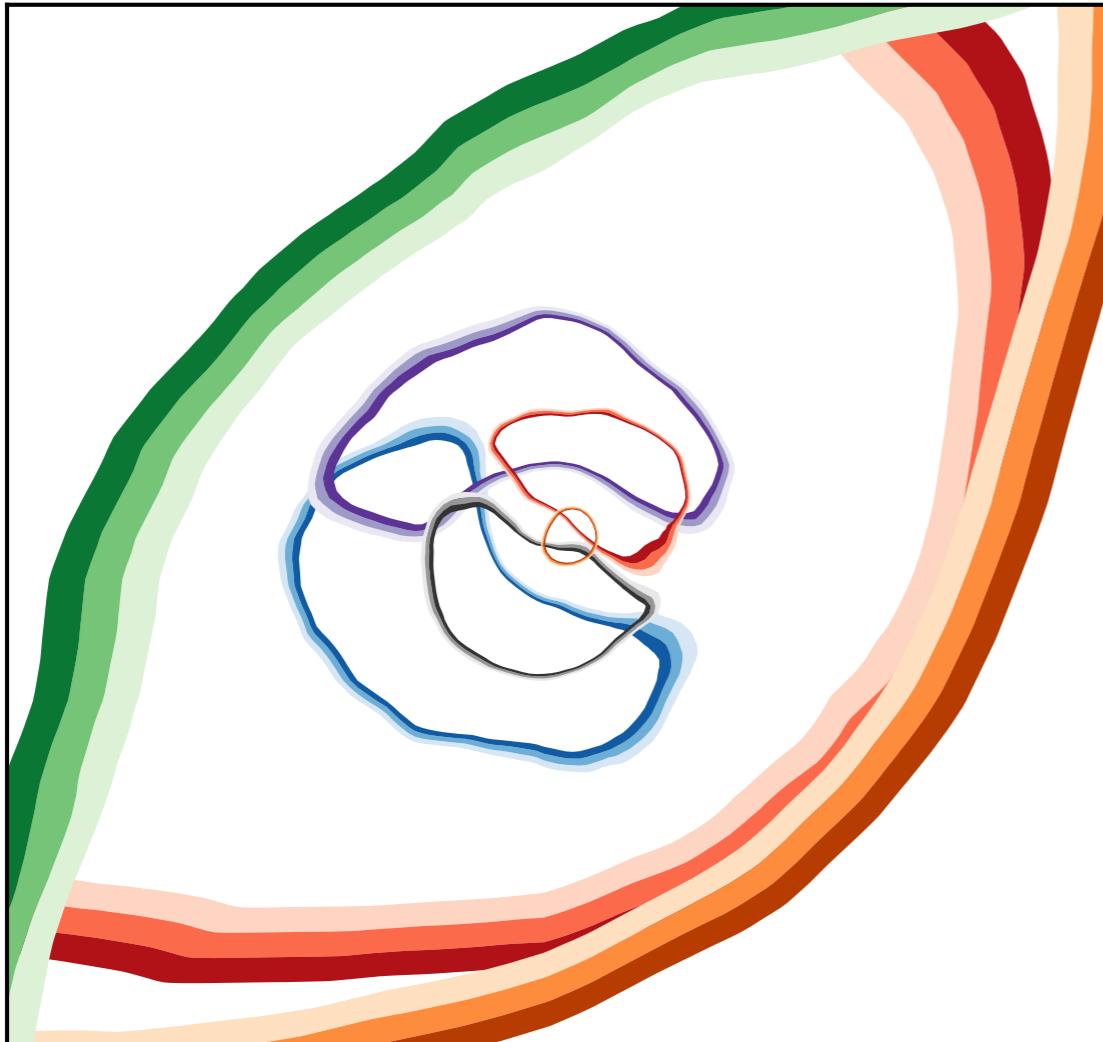


Overlay

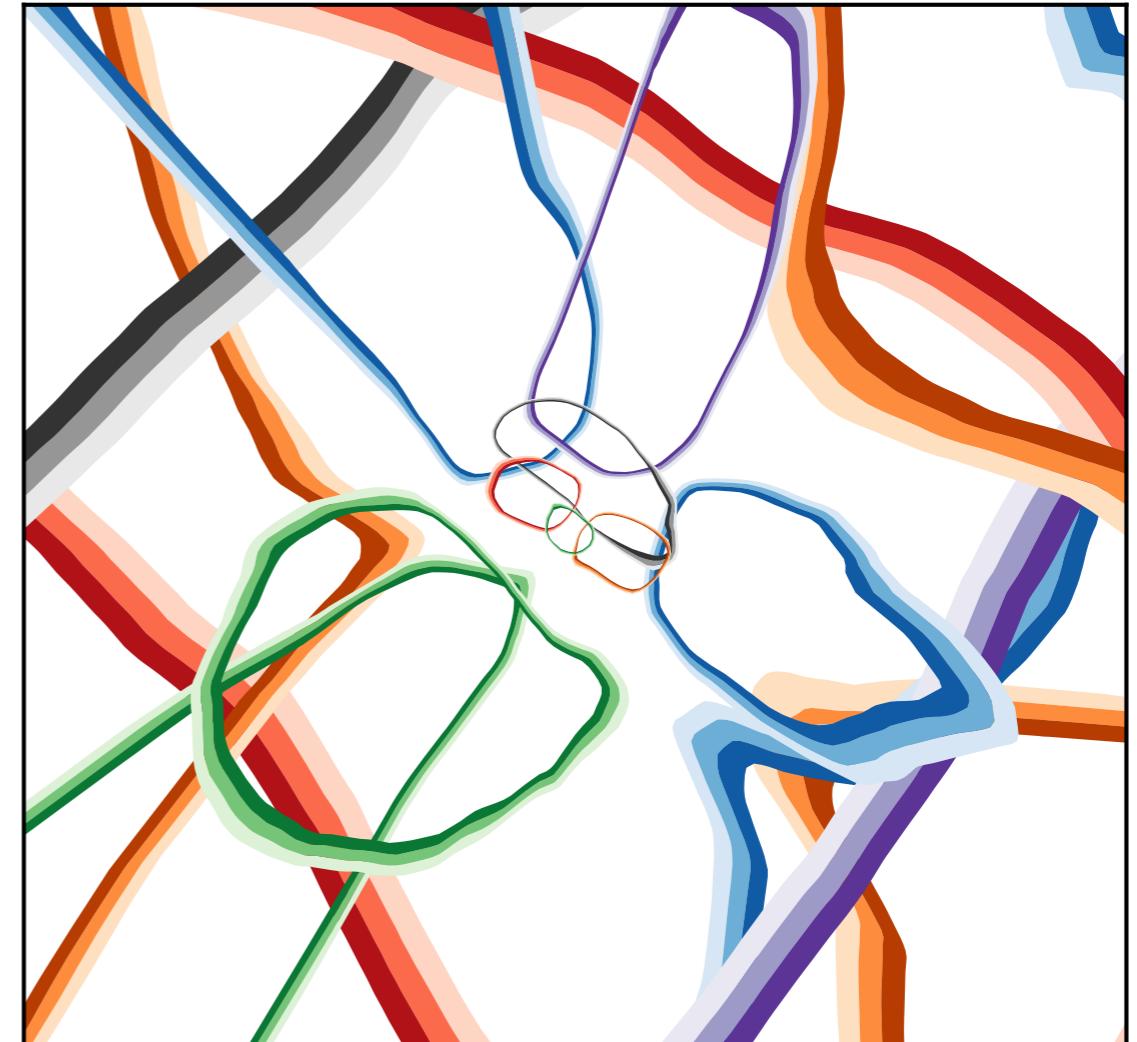


Psychedelic Network Visualization

Latent Dimension 8

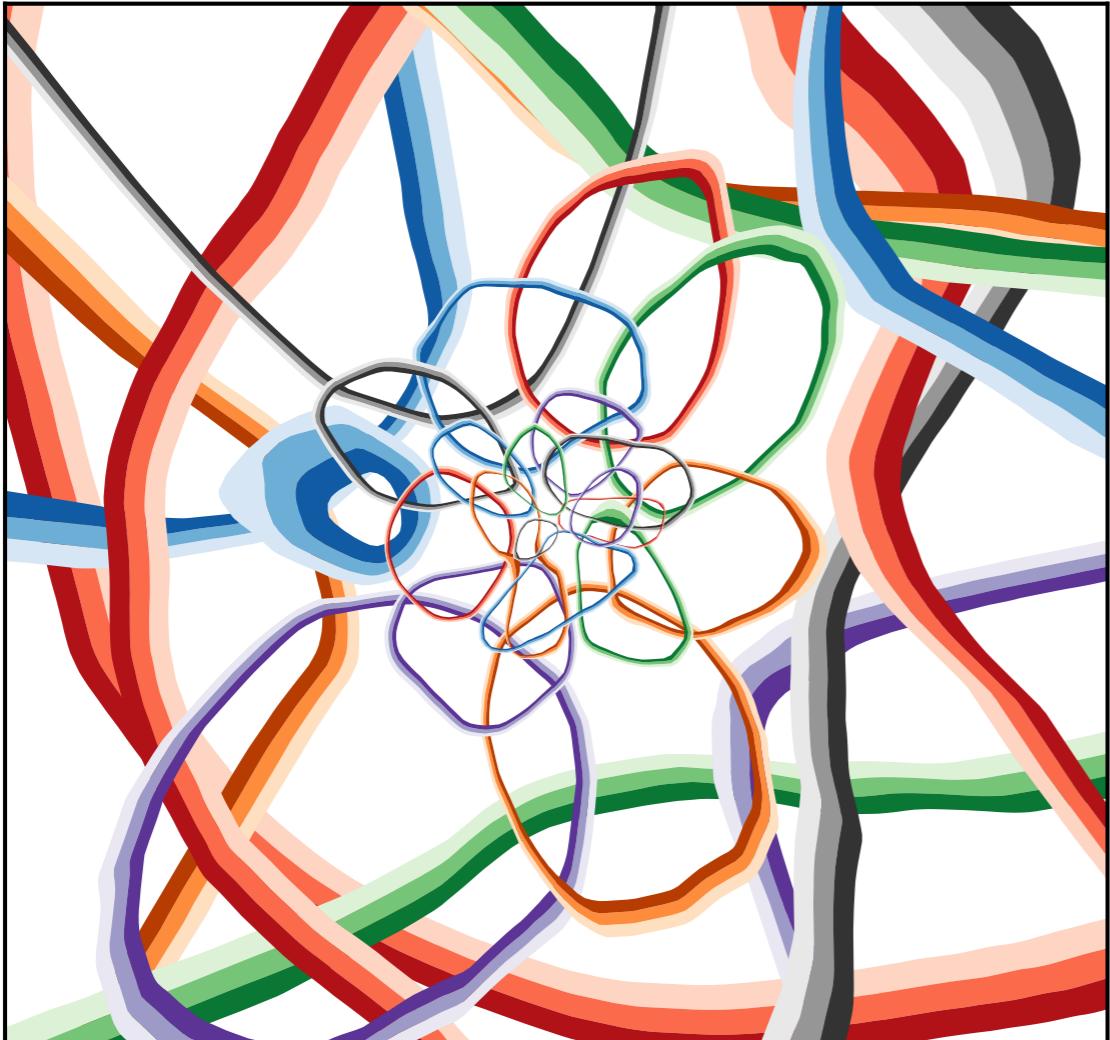


Latent Dimension 16



Psychedelic Network Visualization

Latent Dimension 32

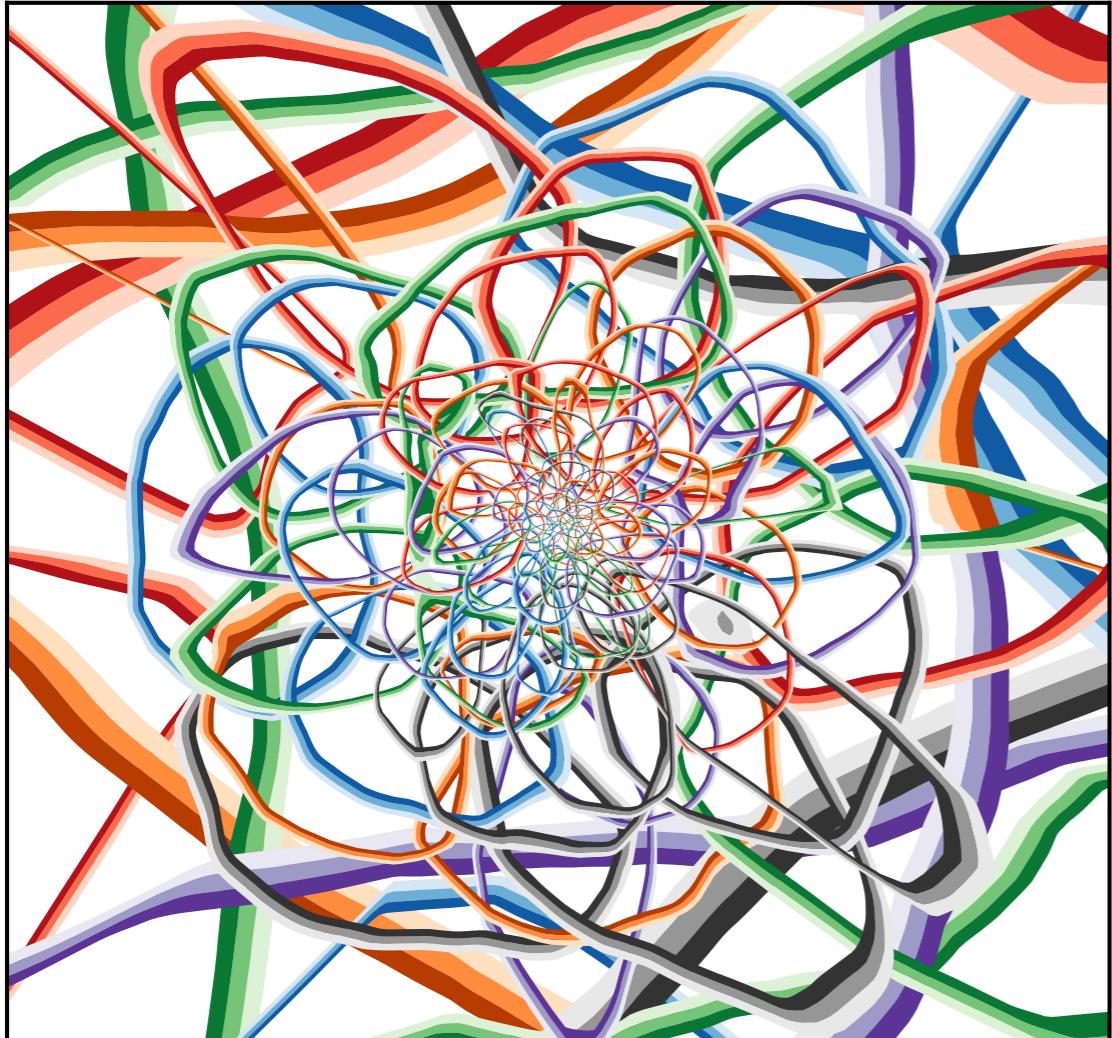


Latent Dimension 64

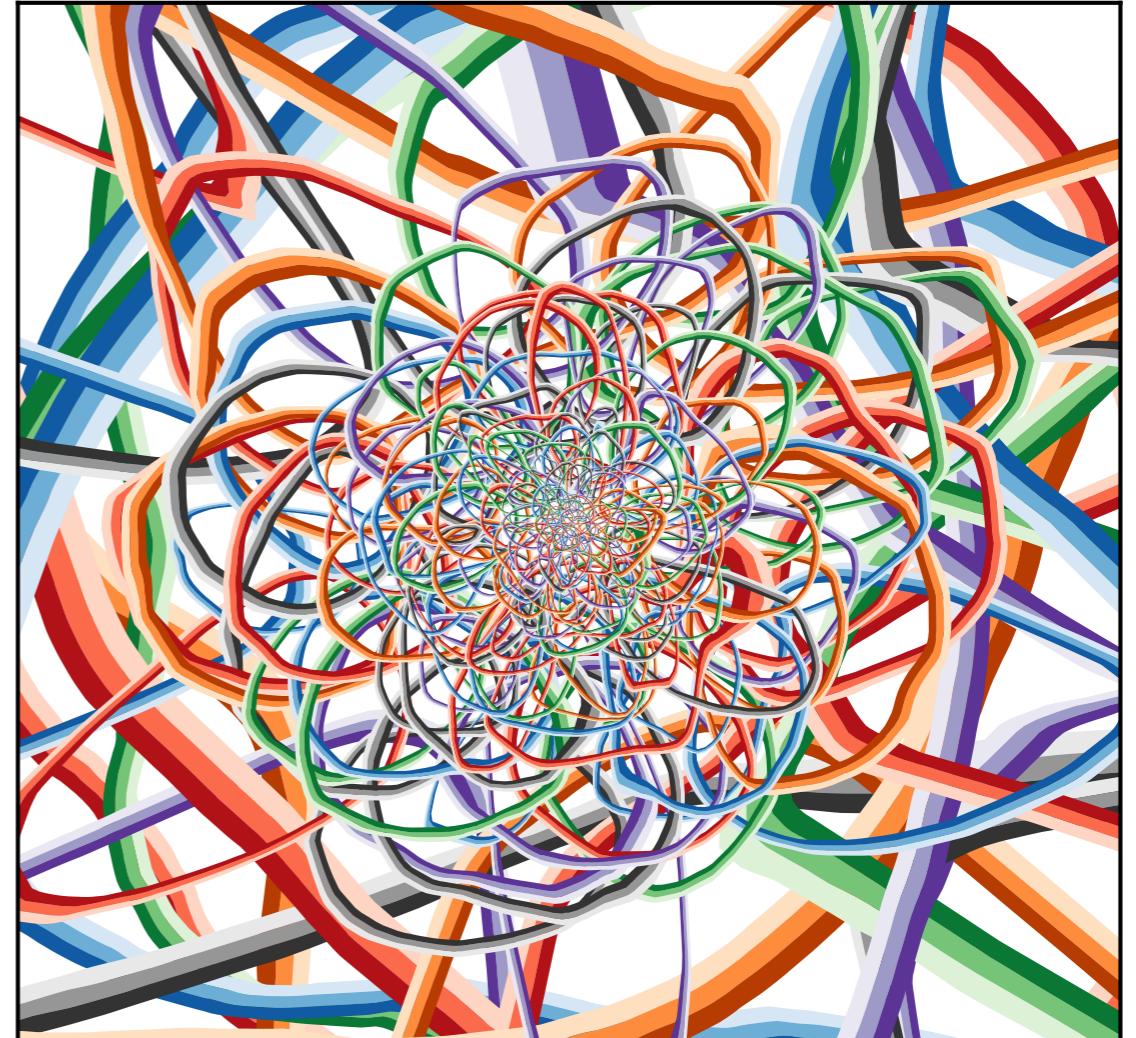


Psychedelic Network Visualization

Latent Dimension 128

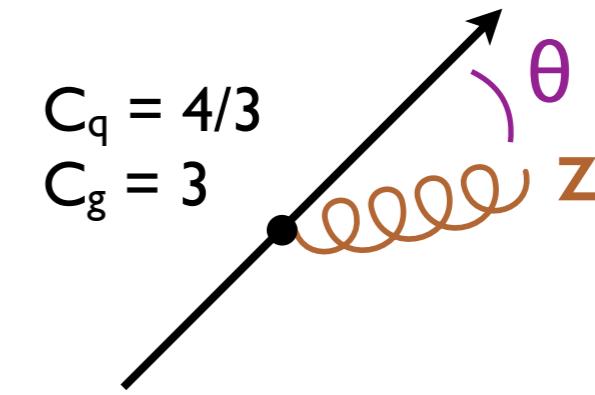
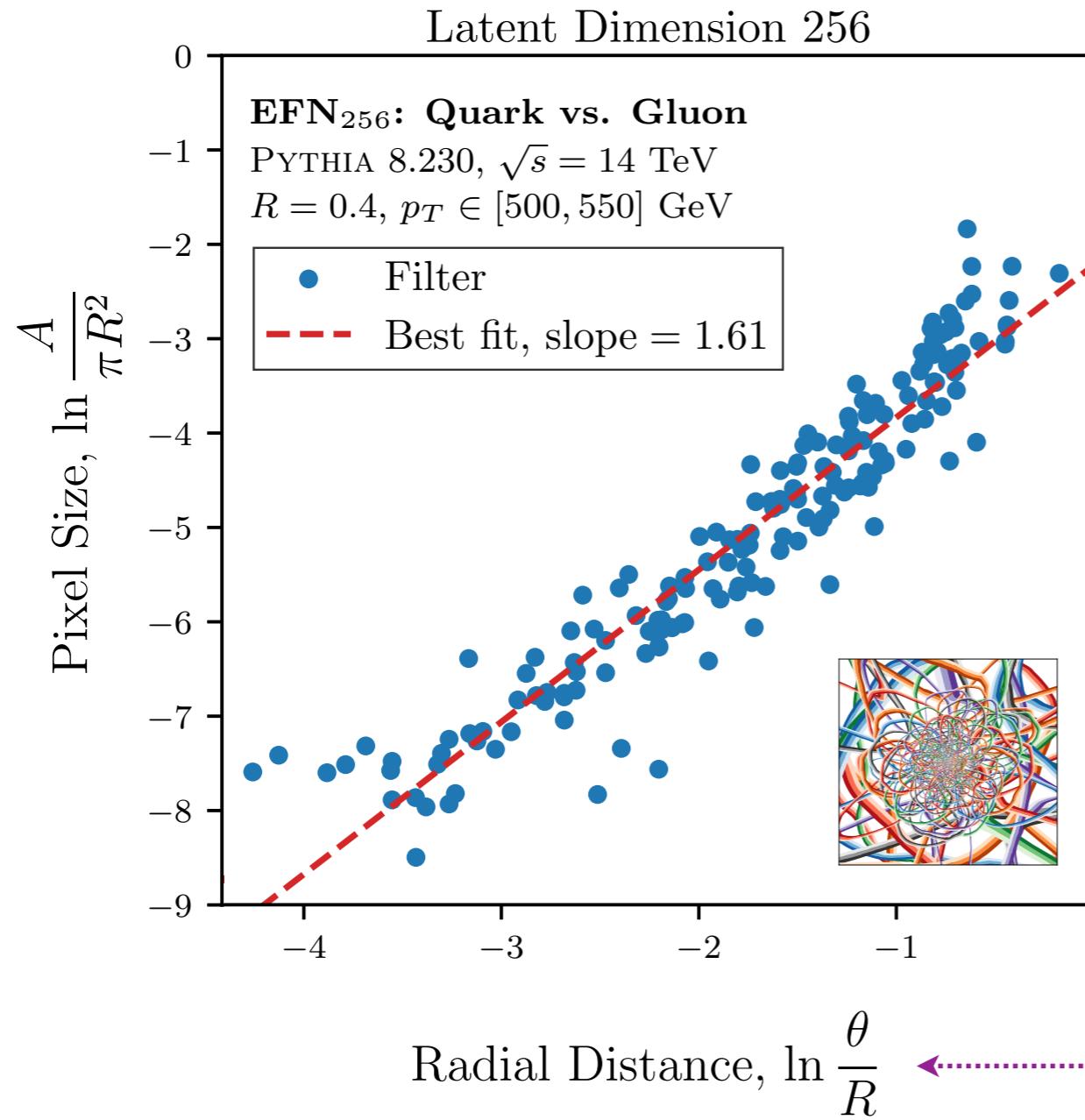


Latent Dimension 256



Altarelli-Parisi!

Learning the Structure of QCD



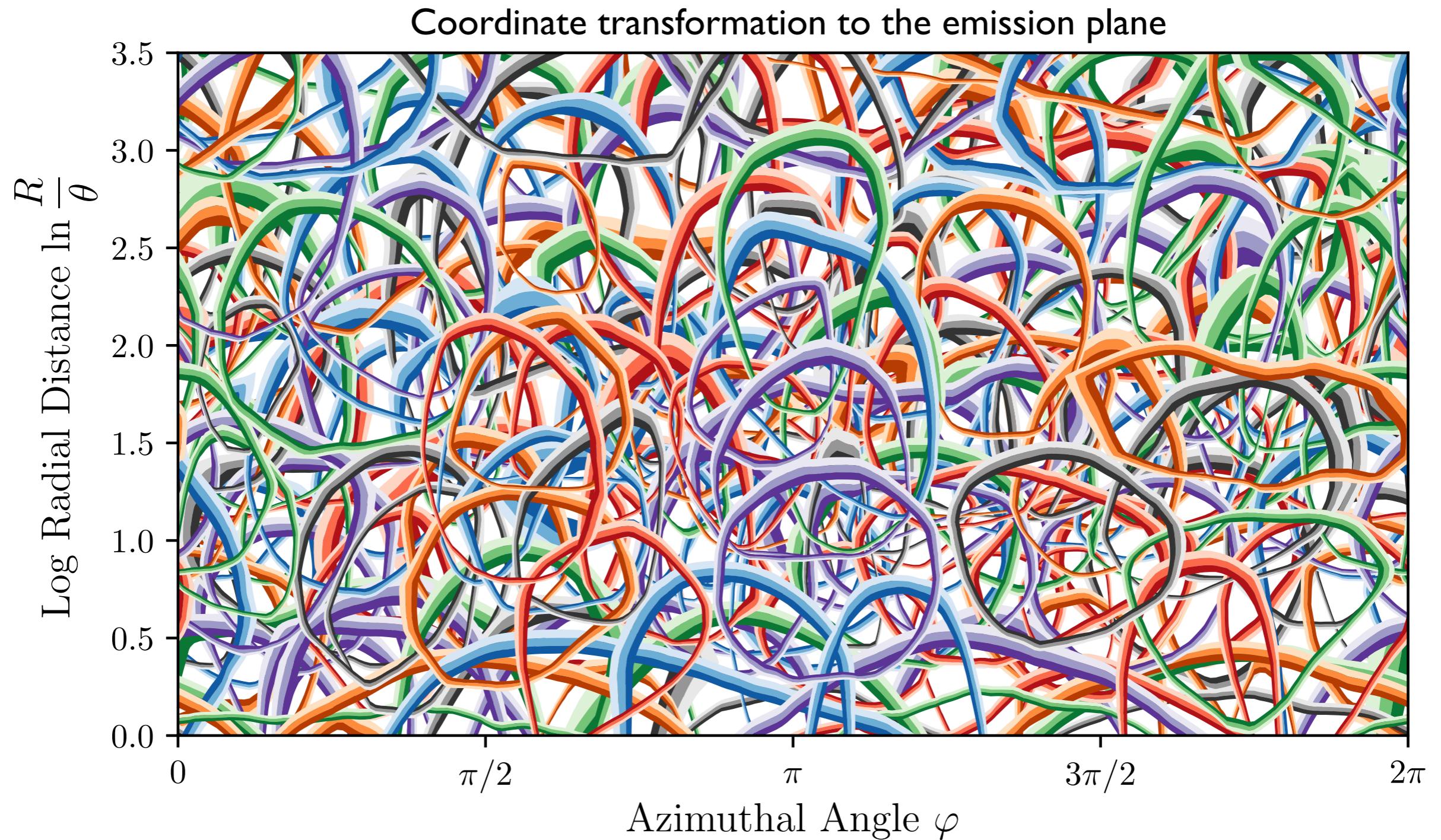
$$dP_{i \rightarrow ig} \sim \frac{2\alpha_s}{\pi} C_i \frac{d\theta}{\theta} \frac{dz}{z}$$

Collinear Soft

A dotted purple arrow points from the text "Collinear" to the purple bracket under the $d\theta/\theta$ term, and another dotted orange arrow points from the text "Soft" to the orange bracket under the dz/z term.

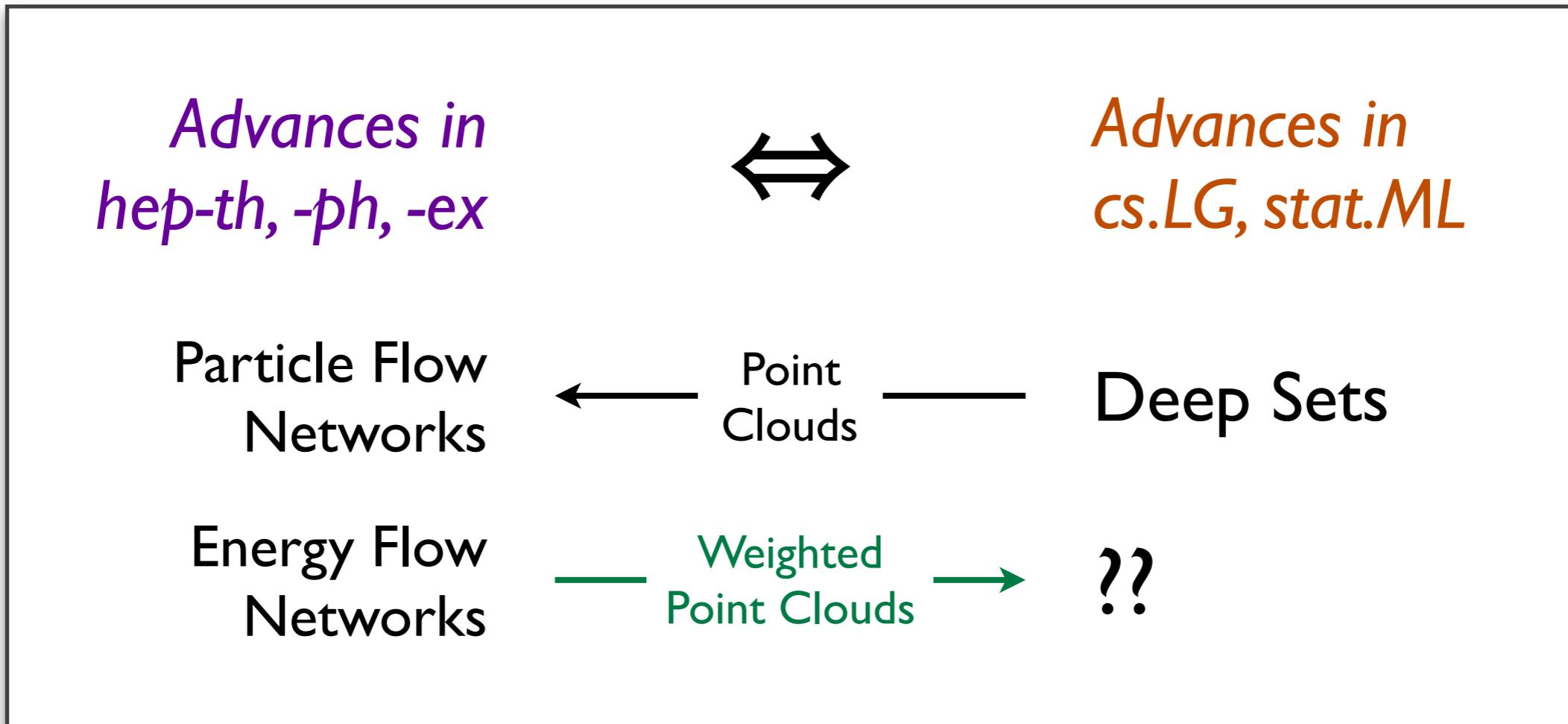
[Komiske, Metodiev, JDT, 1810.05165]

Ready for the SFMOMA?



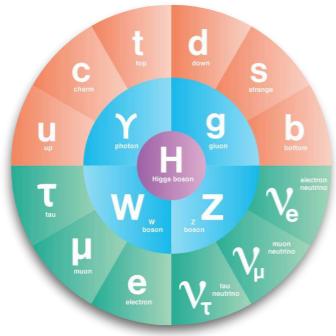
[Komiske, Metodiev, JDT, 1810.05165]

“Collision Course”



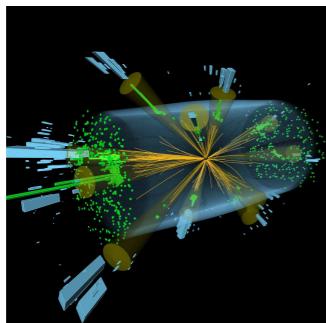
Particle physics is a fascinating domain with rich data sets, established algorithms, and strong theory foundations

Summary



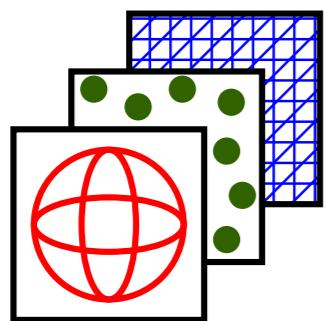
Particle Physics Primer

A rich domain with many machine learning opportunities



Jets and Point Clouds

The importances of symmetries (and safety)



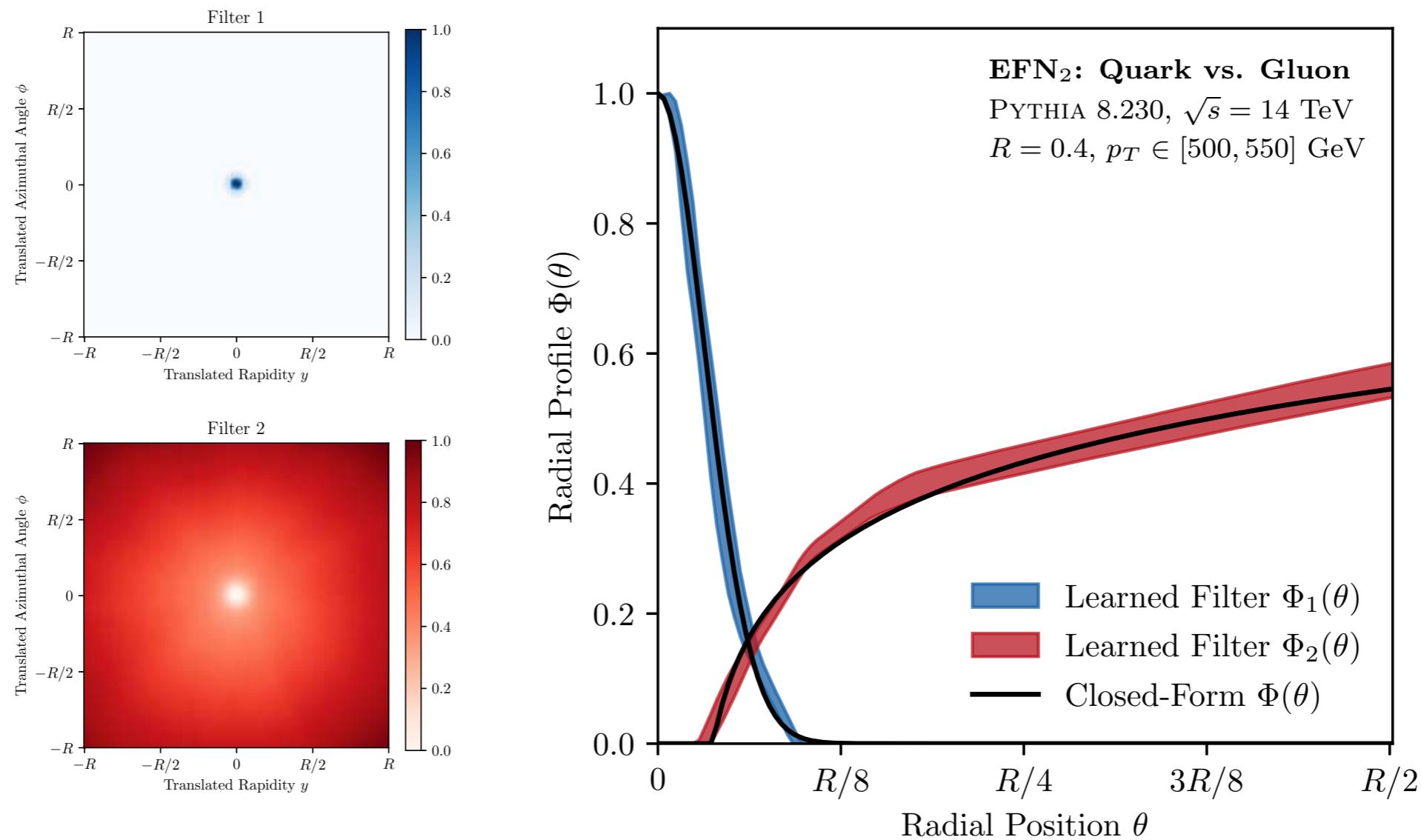
Energy Flow Networks

A new architecture for weighted point clouds

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

Learning from the Machine

For $\ell = 2$ EFN, radial moments: $\sum_{i \in \text{jet}} z_i f(\theta_i)$ cf. Angularities:
 $f(\theta) = \theta^\beta$

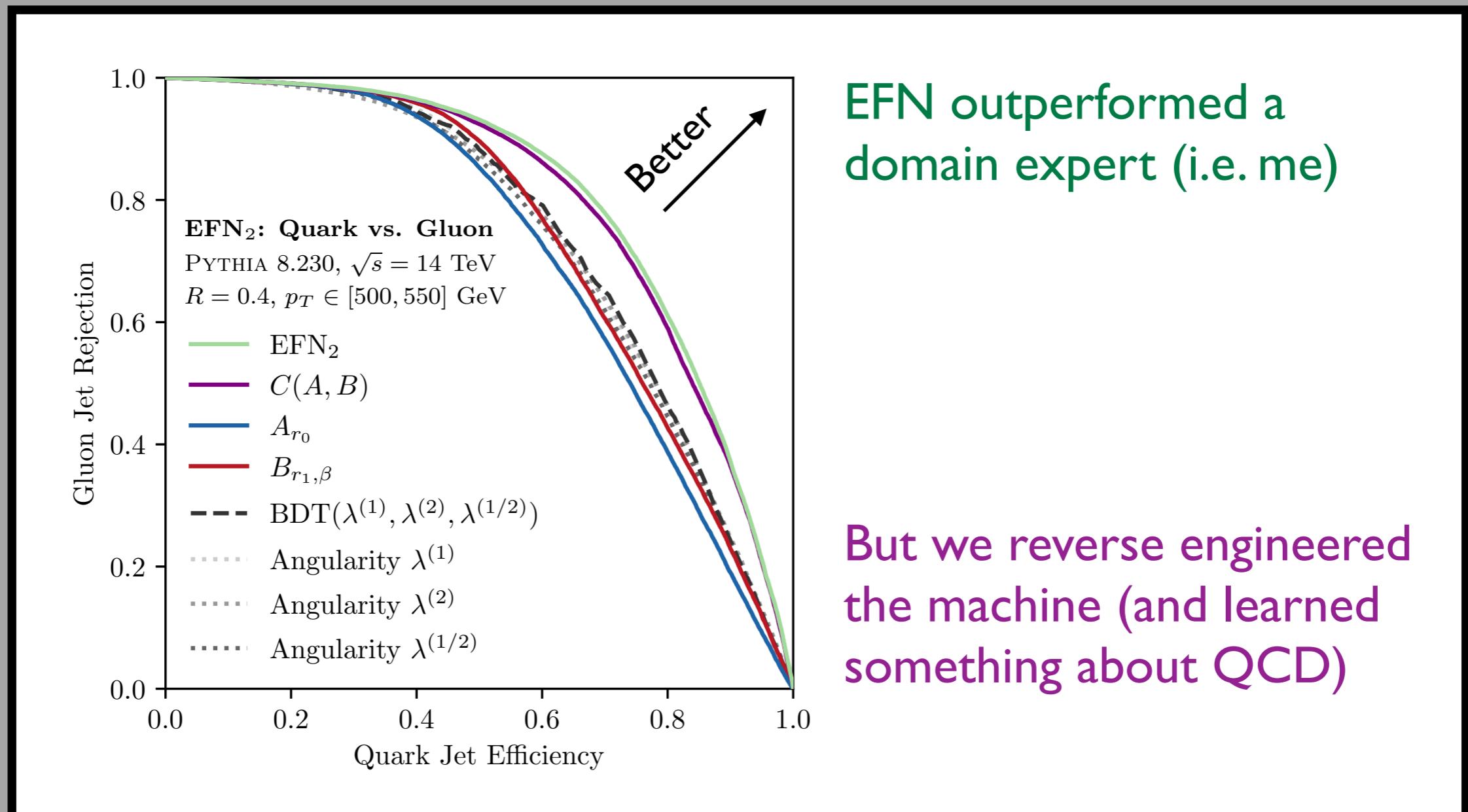


Learning from the Machine

For $\ell = 2$ EFN, radial moments:

$$\sum_{i \in \text{jet}} z_i f(\theta_i)$$

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



(Theoretical)
Particle
Physics



Patrick Komiske



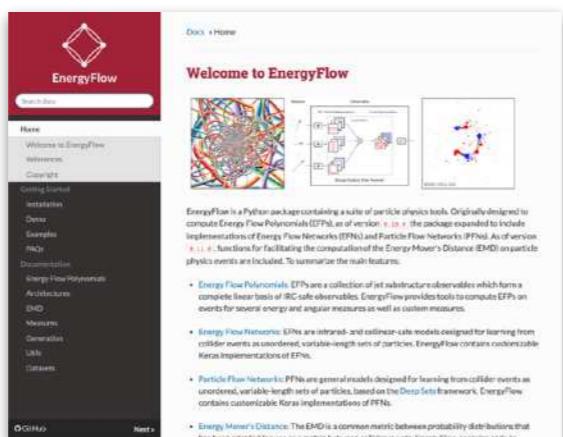
Eric Metodiev



Thank you!



Mathematics,
Statistics,
Computer Science



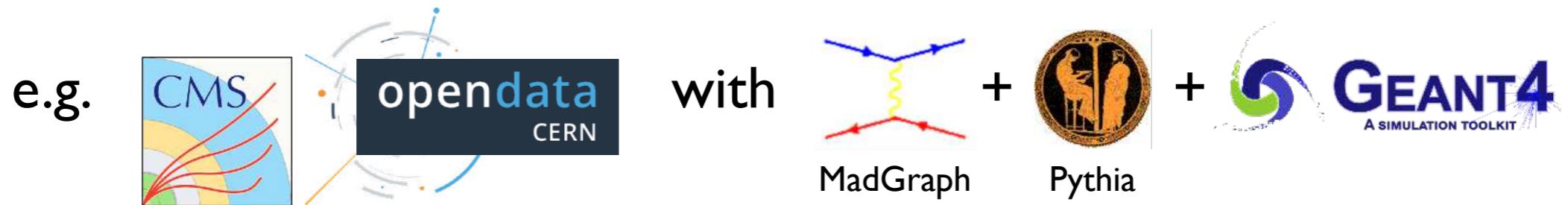
Energy Flow Networks

<https://energyflow.network/>

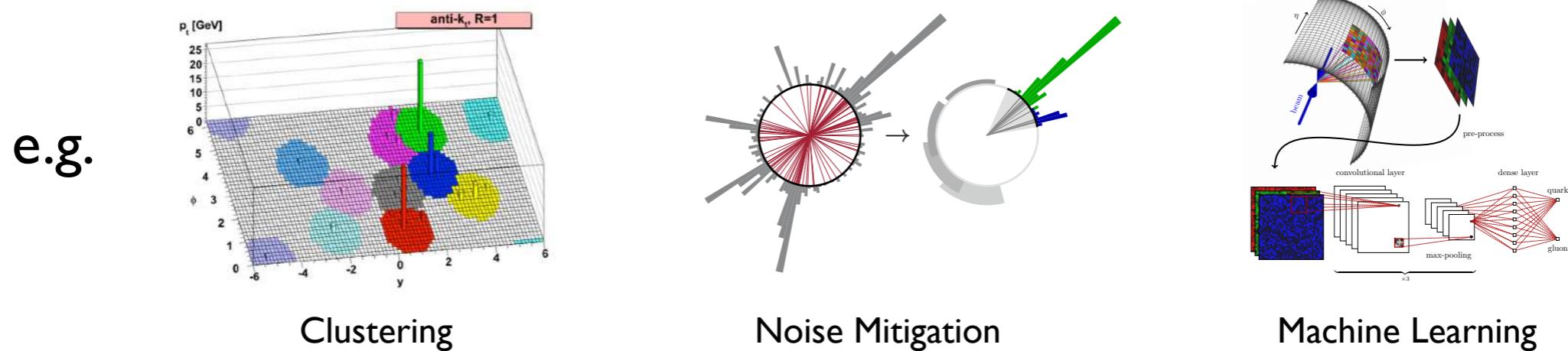
Backup Slides

Particle Physics as ML Testbed

- Huge datasets with reliable simulations

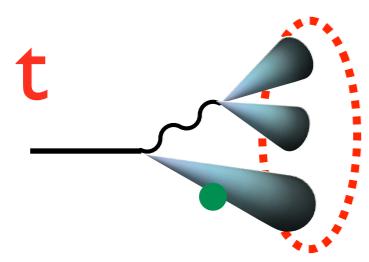


- Broad use of (un)supervised algorithms

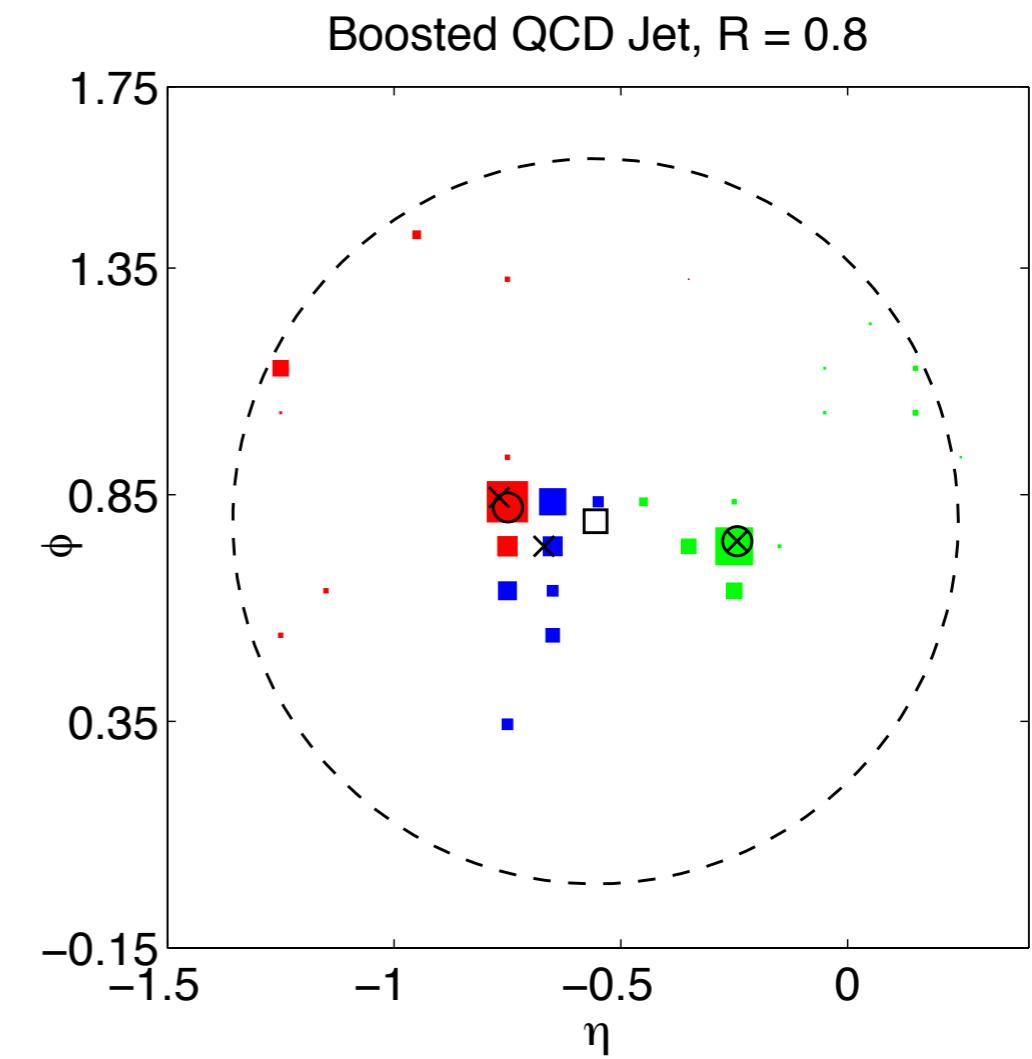
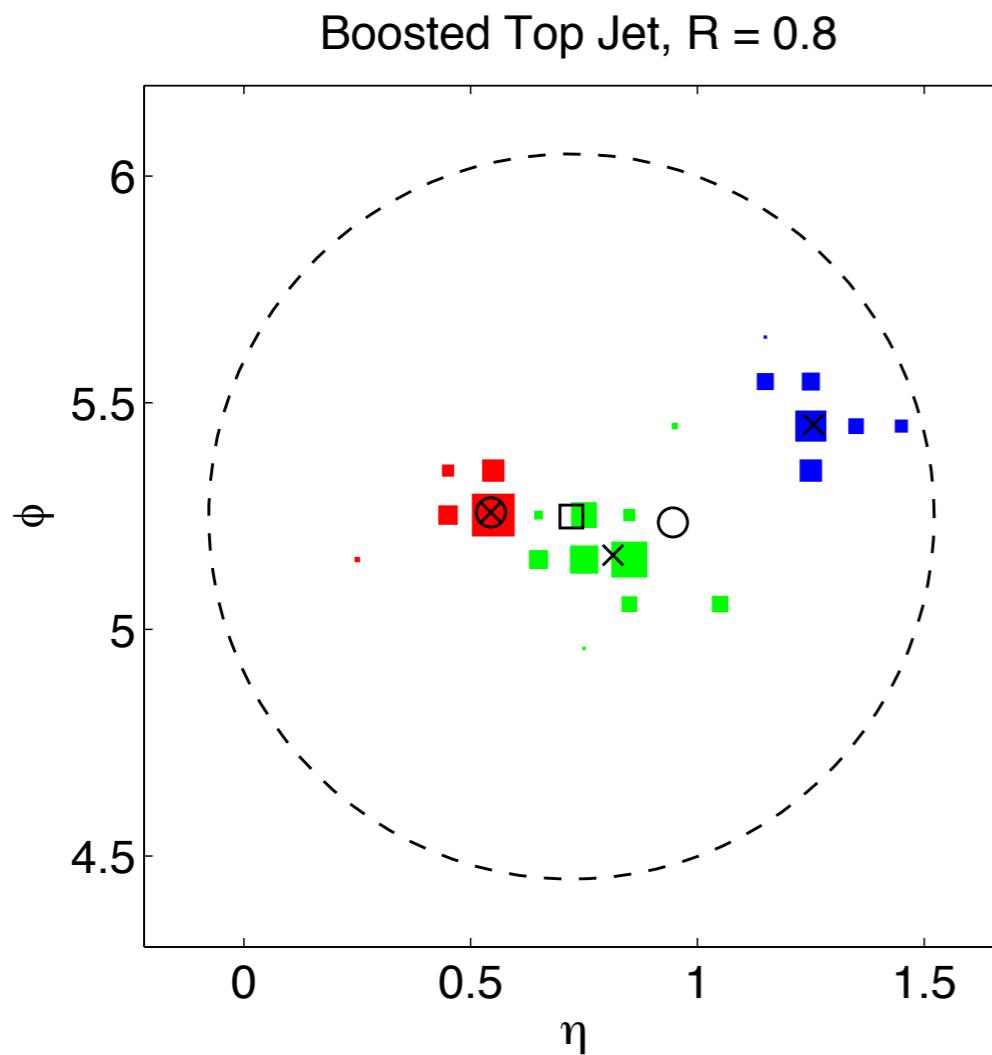
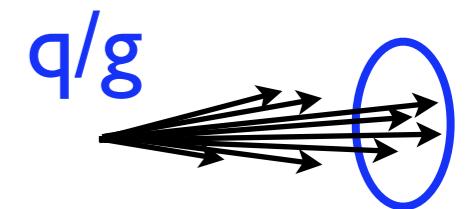


- Extensive domain knowledge and strong theory foundations

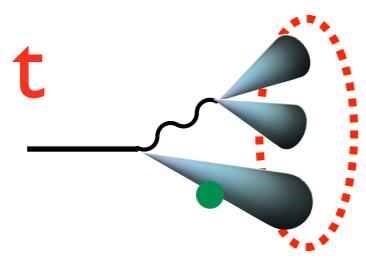
[figures from Cacciari, Salam, Soyez, [0802.1189](#); Larkoski, Marzani, JDT, Tripathee, Xue, [1704.05066](#); Komiske, Metodiev, Schwartz, [1612.01551](#)]



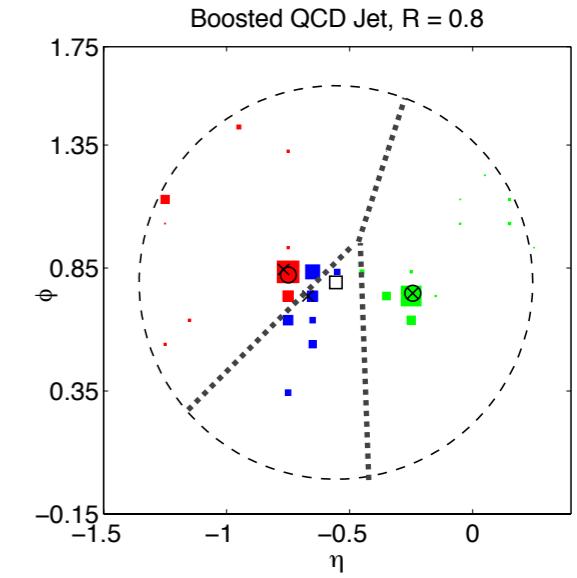
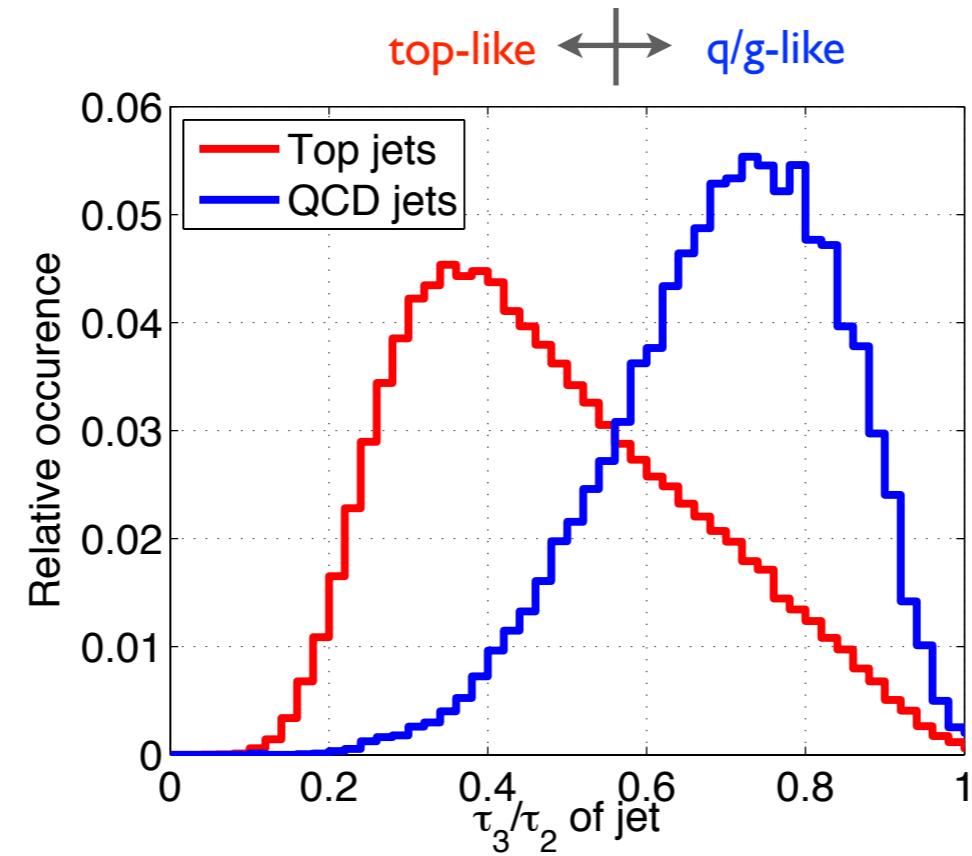
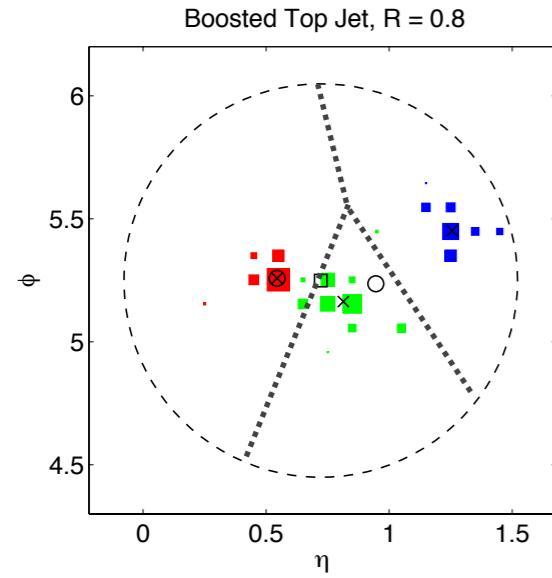
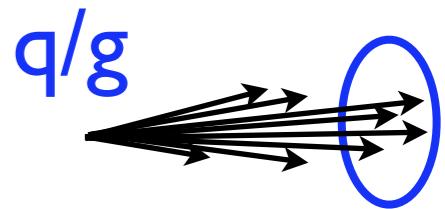
3-Prong vs. 1-Prong



If your eyes can do it...



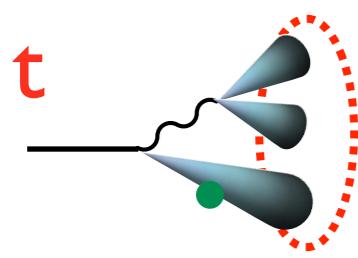
3-Prong vs. 1-Prong



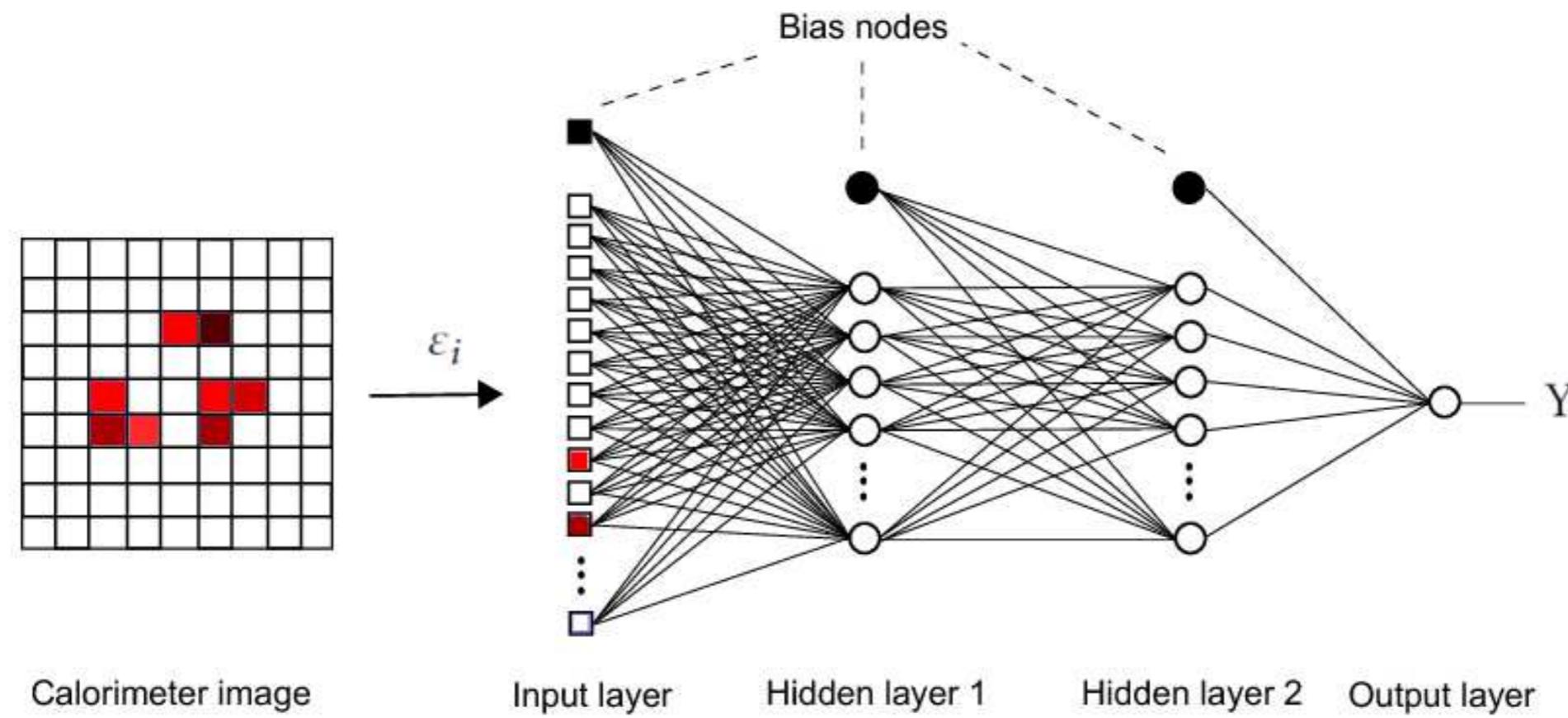
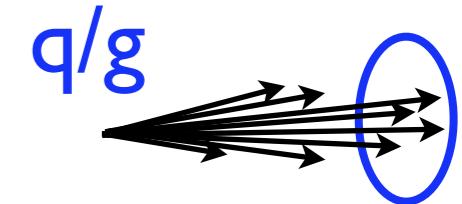
“Deep Thinking”: *N-subjettiness*

$$\tau_N(\mathcal{J}) = \min_{|\mathcal{J}'|=N} \text{EMD}(\mathcal{J}, \mathcal{J}')$$

[JDT, Van Tilburg, [1011.2268](#), [1108.2701](#);
rephrased in language of Komiske, Metodiev, JDT, [1902.02346](#)]



3-Prong vs. 1-Prong



“Deep Learning”:

**BDT, FLD, DNN, CNN, P-CNN,
RNN, RecNN, LBN, LoLa, DGCNN,
EFP, PFN, EFN, ResNeXT, ...**

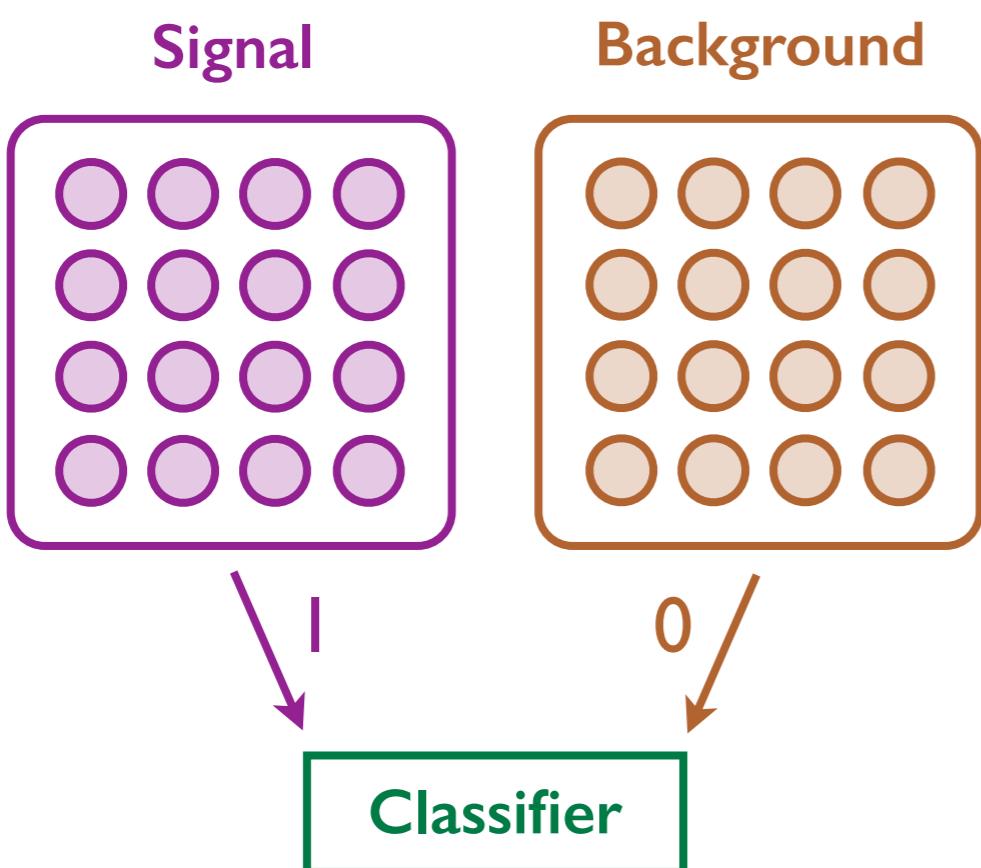
[figure from Almeida, Backović, Cliche, Lee, Perelstein, [1501.05968](#);
head to head comparison in Kasieczka, Plehn, et al. ([Komiske, Metodiev](#)), [1902.09914](#)]

A Cartoon of Machine Learning

For fully-supervised jet classification

$$\ell_{\text{MSE}} = \left\langle (\textcolor{teal}{h}(\vec{x}) - 1)^2 \right\rangle_{\text{signal}} + \left\langle (\textcolor{teal}{h}(\vec{x}) - 0)^2 \right\rangle_{\text{background}}$$

Classifier Inputs



Minimize Loss Function

(assuming infinite training sets,
and flexible enough functional form)

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

Optimal Classifier (Neyman–Pearson)

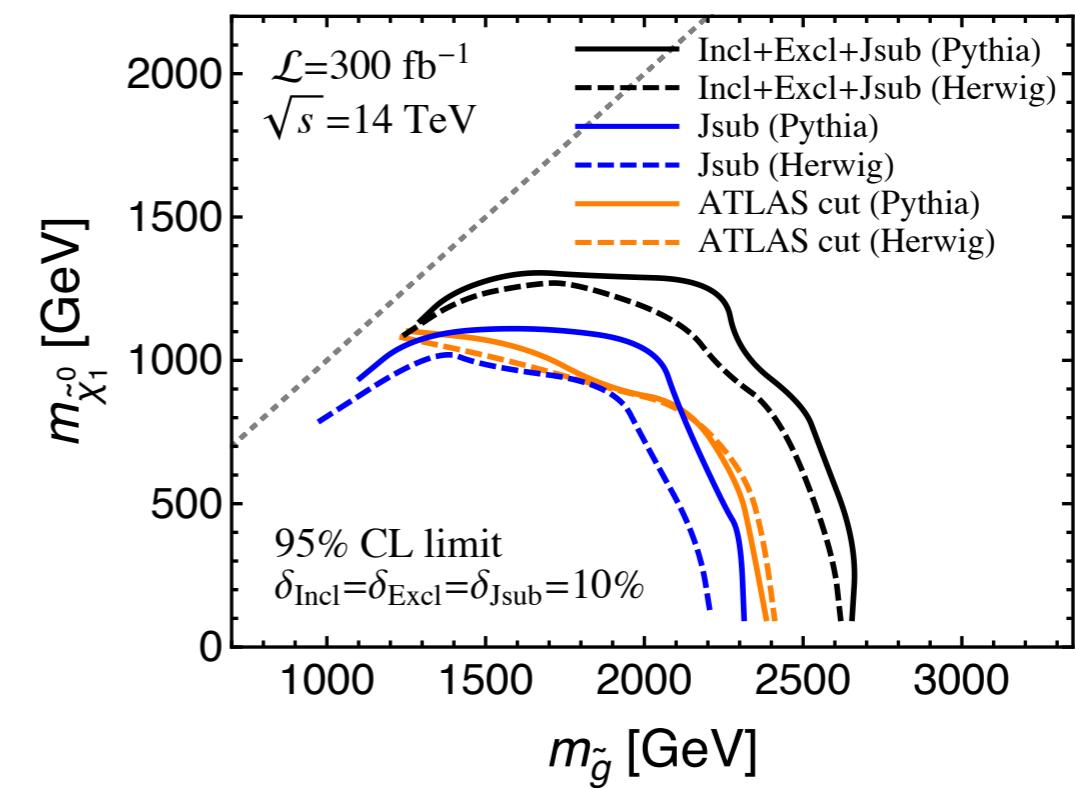
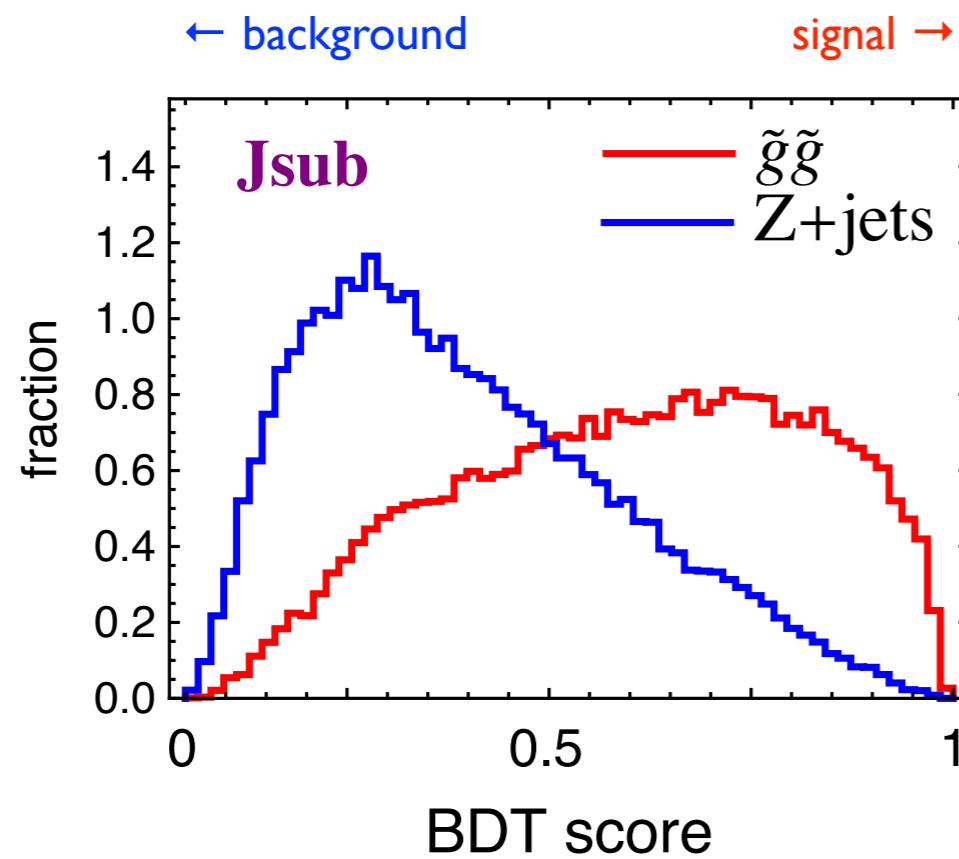
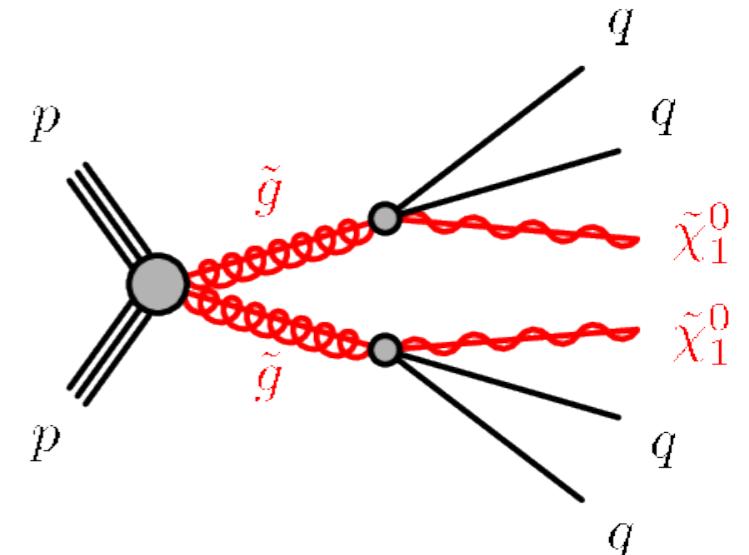
E.g. Search for Gluino Cascade to Dark Matter

Classifier: Boosted decision tree (for each of 4 jets)

Inputs: Jet mass, width, track multiplicity

Signal: Quark enriched ($C_F = 4/3$)

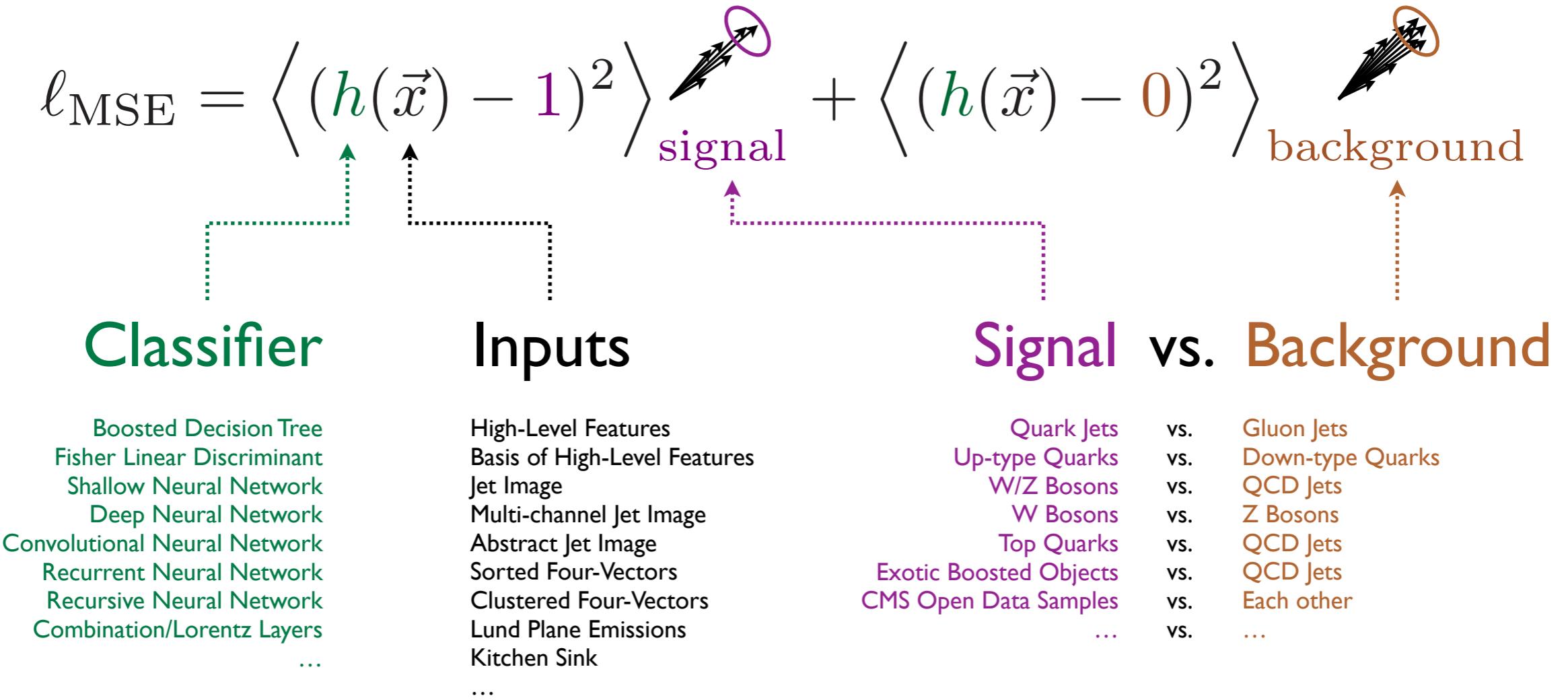
Background: Gluon enriched ($C_A = 3$)



[Bhattacherjee, Mukhopadhyay, Nojiri, Sakakie, Webber, 1609.08781]

Jet Classification Studies

Mix and match



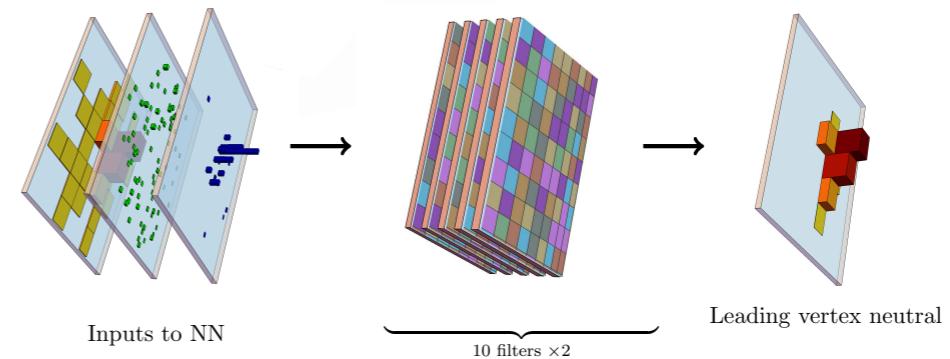
[Lönnblad, Peterson, Rögnvaldsson, 1990, ..., Cogan, Kagan, Strauss, Schwartzman, 1407.5675; Almeida, Backović, Cliche, Lee, Perelstein, 1501.05968; de Oliveira, Kagan, Mackey, Nachman, Schwartzman, 1511.05190; Baldi, Bauer, Eng, Sadowski, Whiteson, 1603.09349; Conway, Bhaskar, Erbacher, Pilot, 1606.06859; Guest, Collado, Baldi, Hsu, Urban, Whiteson, 1607.08633; Barnard, Dawe, Dolan, Rajcic, 1609.00607; Komiske, Metodiev, Schwartz, 1612.01551; Kasieczka, Plehn, Russell, Schell, 1701.08784; Louppe, Cho, Becot, Cranmer, 1702.00748; Pearkes, Fedorko, Lister, Gay, 1704.02124; Datta, Larkoski, 1704.08249, 1710.01305; Butter, Kasieczka, Plehn, Russell, 1707.08966; Fernández Madrazo, Heredia Cacha, Lloret Iglesias, Marco de Lucas, 1708.07034; Aguilar Saavedra, Collin, Mishra, 1709.01087; Cheng, 1711.02633; Luo, Luo, Wang, Xu, Zhu, 1712.03634; Komiske, Metodiev, JDT, 1712.07124; Macaluso, Shih, 1803.00107; Fraser, Schwartz, 1803.08066; Choi, Lee, Perelstein, 1806.01263; Lim, Nojiri, 1807.03312; Dreyer, Salam, Soyez, 1807.04758; Moore, Nordström, Varma, Fairbairn, 1807.04769; plus my friends who will scold me for forgetting their paper (and not updating this after July 23, 2018); plus many ATLAS/CMS performance studies]

Beyond Classification

PUMML

Pileup Mitigation

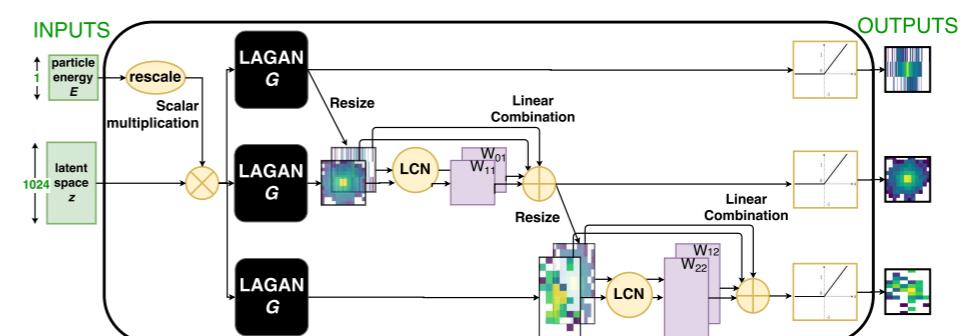
[Komiske, Metodiev, Nachman, Schwartz, 1707.08600]



CaloGAN

Fast Detector Simulation

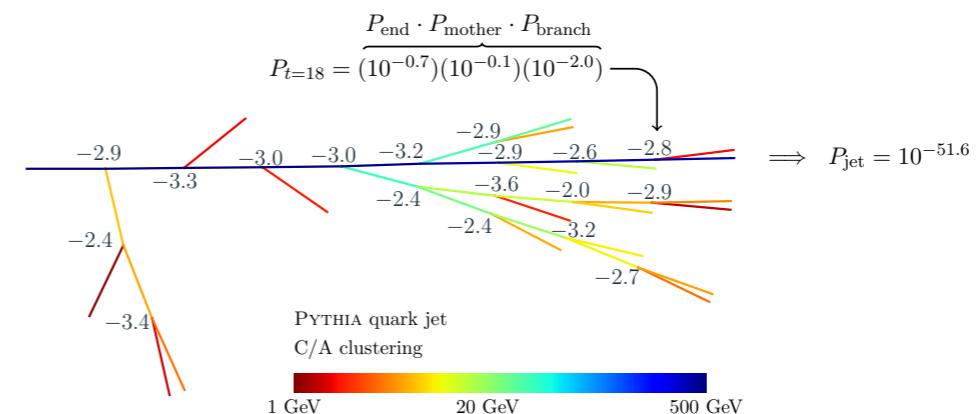
Paganini, de Oliveira, Nachman, 1705.02355, 1712.10321;
see also de Oliveira, Michela Paganini, Nachman, 1701.05927]



JUNIPR

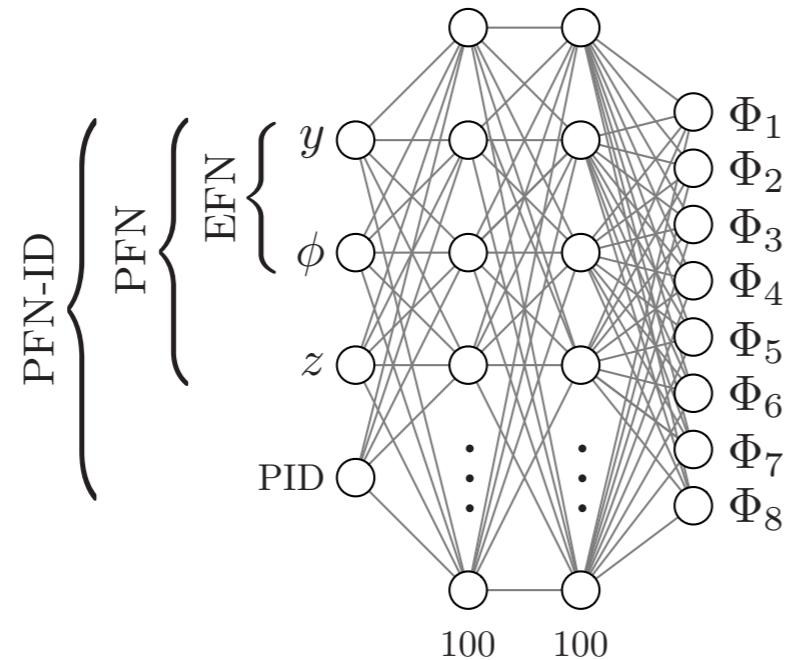
Probability Modeling

[Andreassen, Feige, Frye, Schwartz, 1804.09720;
see also Monk, 1807.03685]



Technical Implementation

Per-Particle Network: Φ

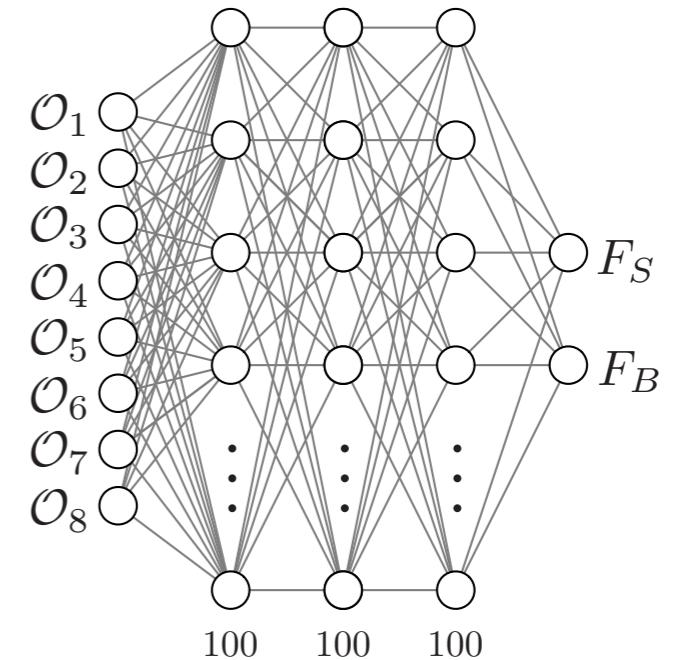


Per-Jet (Latent Space):

$$\text{EFN: } \mathcal{O}_a = \sum_{i \in \text{jet}} z_i \Phi_a(y_i, \phi_i) \quad z_i = \frac{p_{Ti}}{\sum_j p_{Tj}}$$

$$\text{PFN: } \mathcal{O}_a = \sum_{i \in \text{jet}} \Phi_a(y_i, \phi_i, z_i, \text{PID}_i)$$

Latent Combiner: F



Final Discriminant:

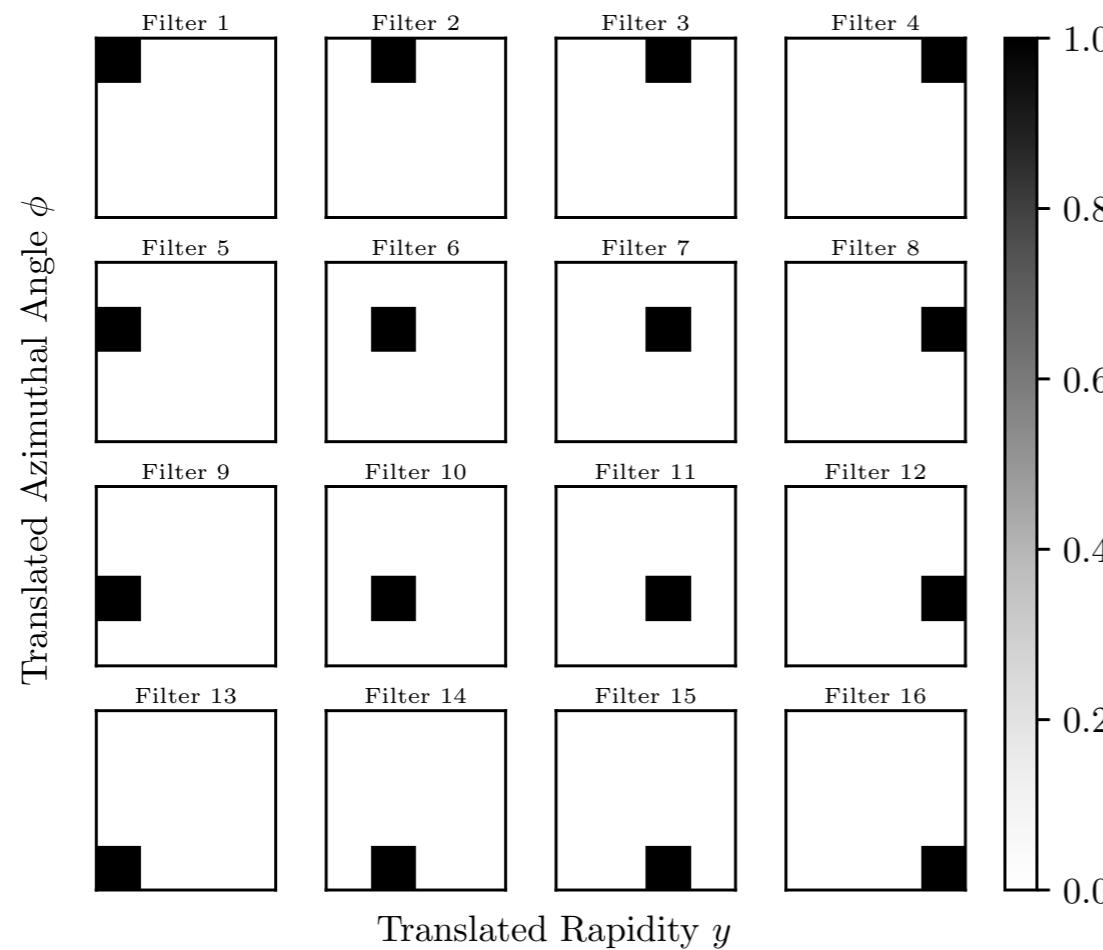
$$\text{softmax}(F_S, F_B)$$

Latent Space Visualization

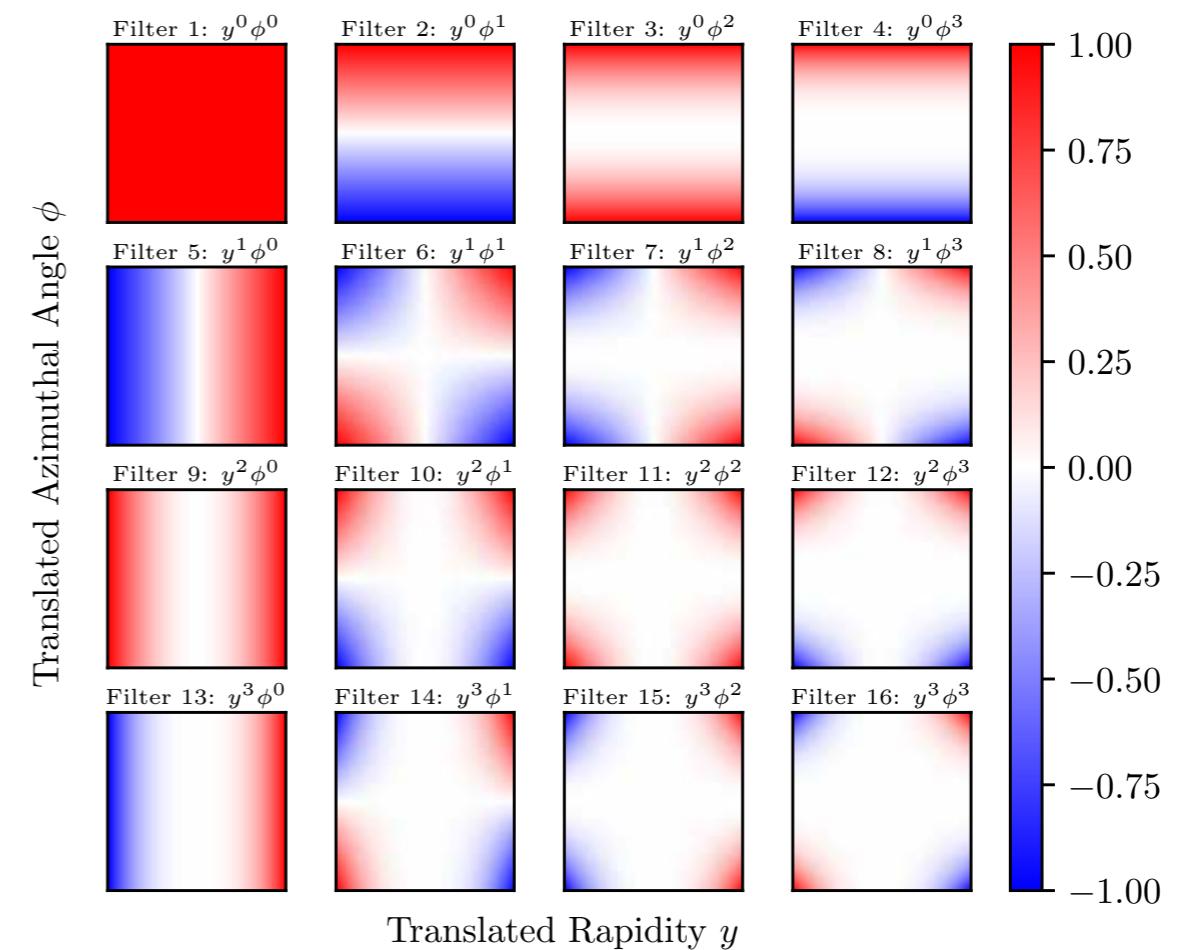
$$\mathcal{O}(\{p_i^\mu\}) = F(\mathcal{O}_1, \mathcal{O}_2, \dots, \mathcal{O}_\ell)$$

IRC-safe: $\mathcal{O}_a = \sum_{i \in \text{jet}} E_i \Phi_a(\hat{p}_i)$

Calorimeter Pixels



Radiation Moments

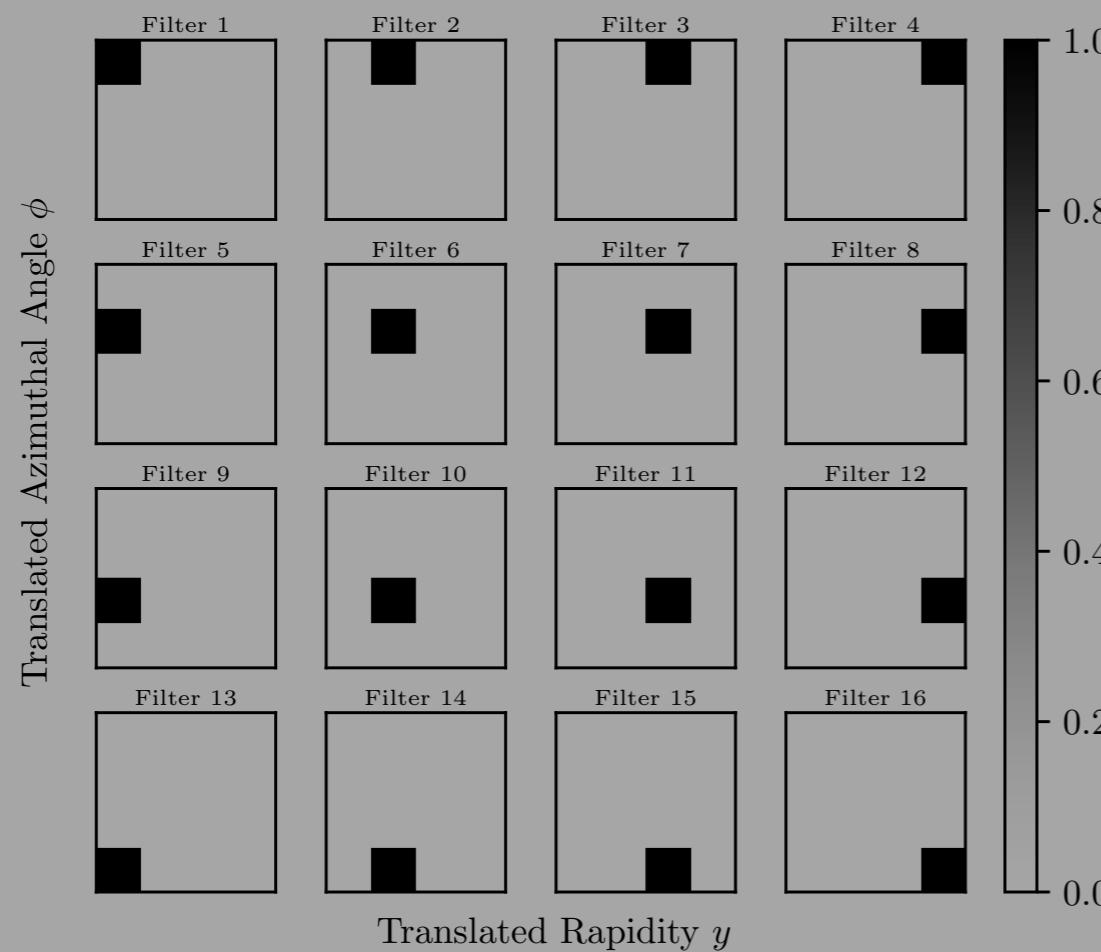


Latent Space Visualization

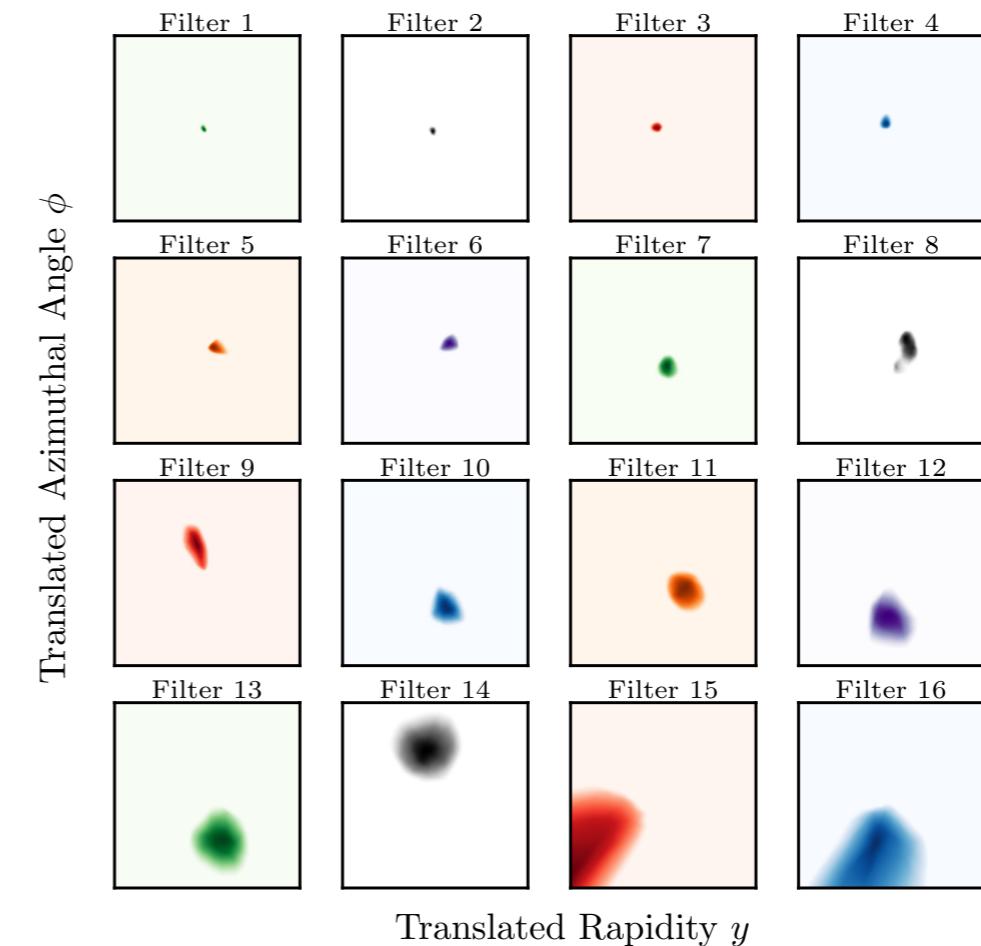
$$\mathcal{O}(\{p_i^\mu\}) = F(\mathcal{O}_1, \mathcal{O}_2, \dots, \mathcal{O}_\ell)$$

IRC-safe: $\mathcal{O}_a = \sum_{i \in \text{jet}} E_i \Phi_a(\hat{p}_i)$

Calorimeter Pixels

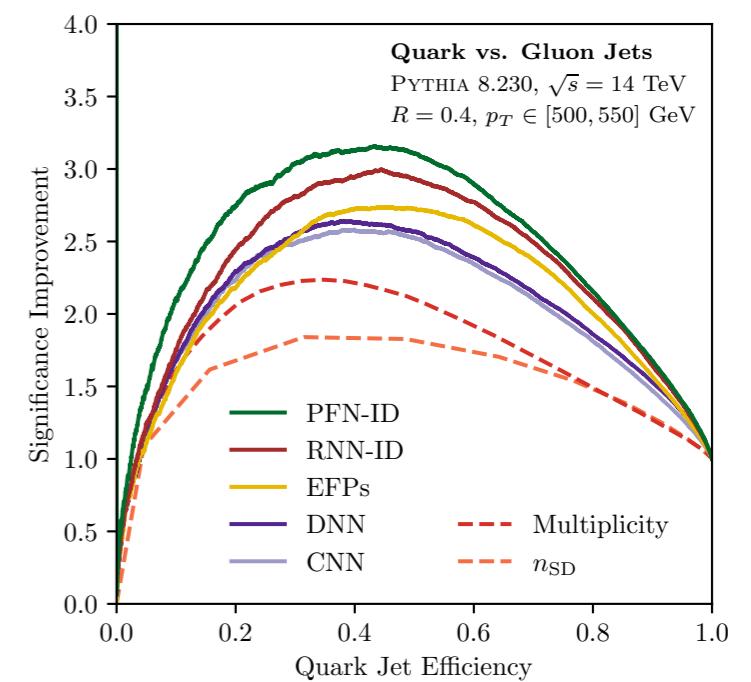
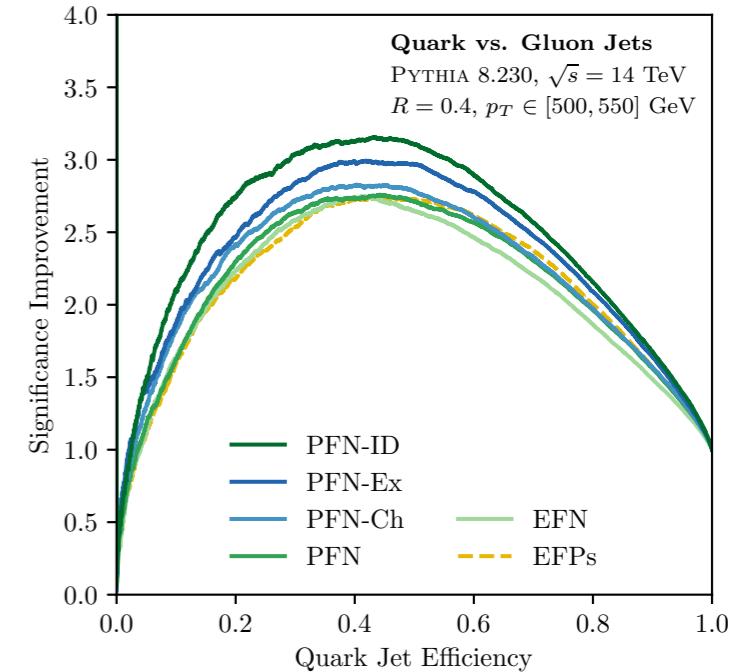


EFNs: Dynamic Pixelation



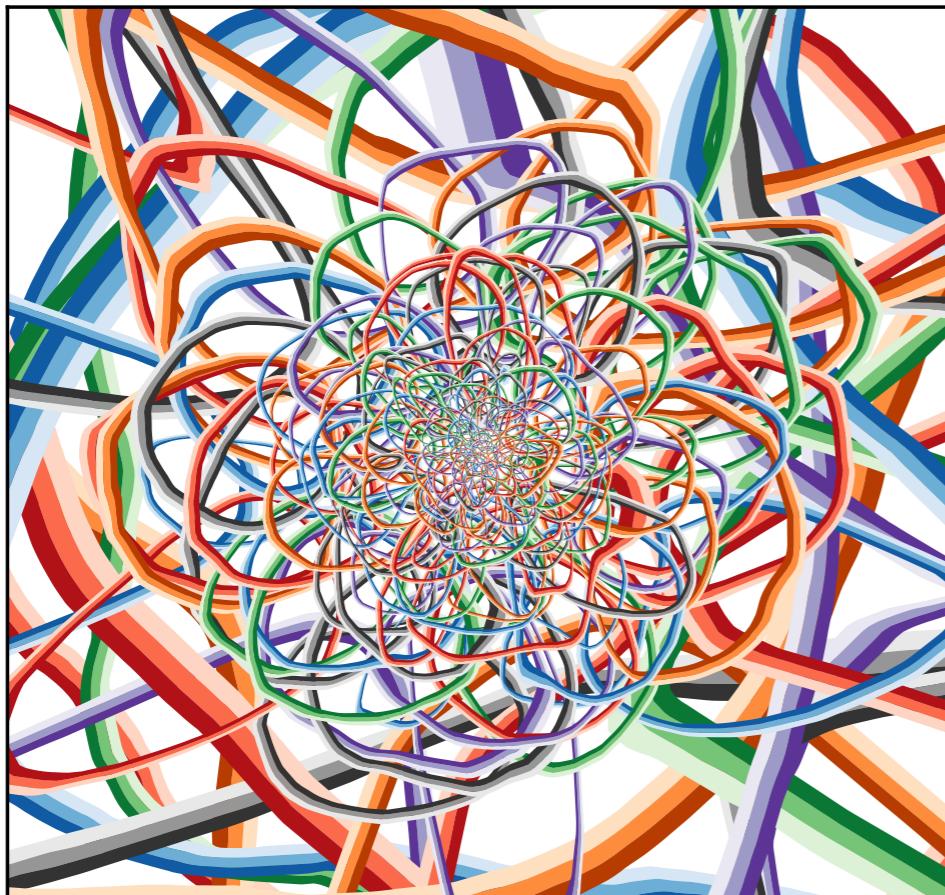
More Quark/Gluon Performance

Model	AUC	$1/\varepsilon_g$ at $\varepsilon_q = 50\%$
PFN-ID	0.9052 ± 0.0007	37.4 ± 0.7
PFN-Ex	0.9005 ± 0.0003	34.7 ± 0.4
PFN-Ch	0.8924 ± 0.0001	31.2 ± 0.3
PFN	0.8911 ± 0.0008	30.8 ± 0.4
EFN	0.8824 ± 0.0005	28.6 ± 0.3
RNN-ID	0.9010	34.4
RNN	0.8899	30.5
EFP	0.8919	29.7
DNN	0.8849	26.4
CNN	0.8781	25.5
M	0.8401	19.0
n_{SD}	0.8297	14.2
m	0.7401	7.2

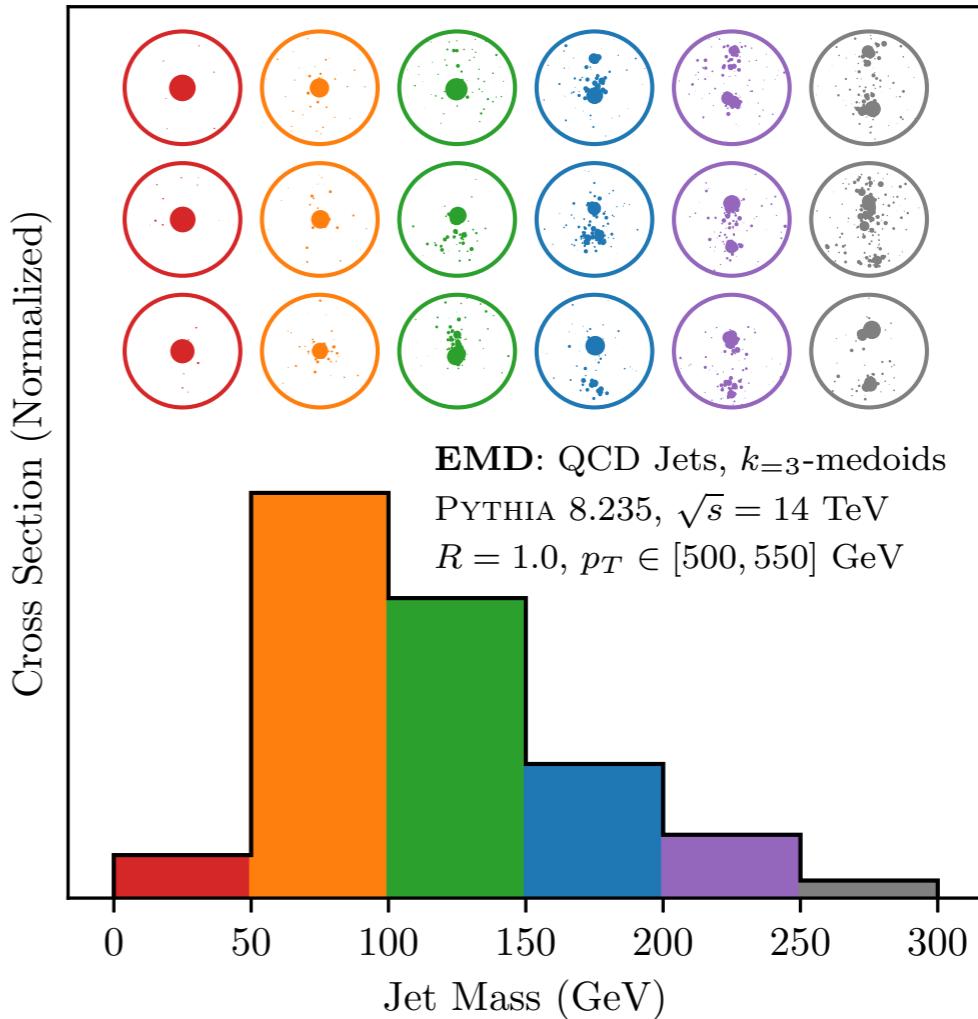


Opportunities for Network/Data Visualization

Latent Space



Metric Space



*Augment (not replace) our exceptional
human/scientific ability to recognize patterns*

[Komiske, Metodiev, JDT, [1810.05165](#); Komiske, Metodiev, JDT, [1902.02346](#)]