# Collision Course

## Particle Physics meets Machine Learning

Jesse Thaler

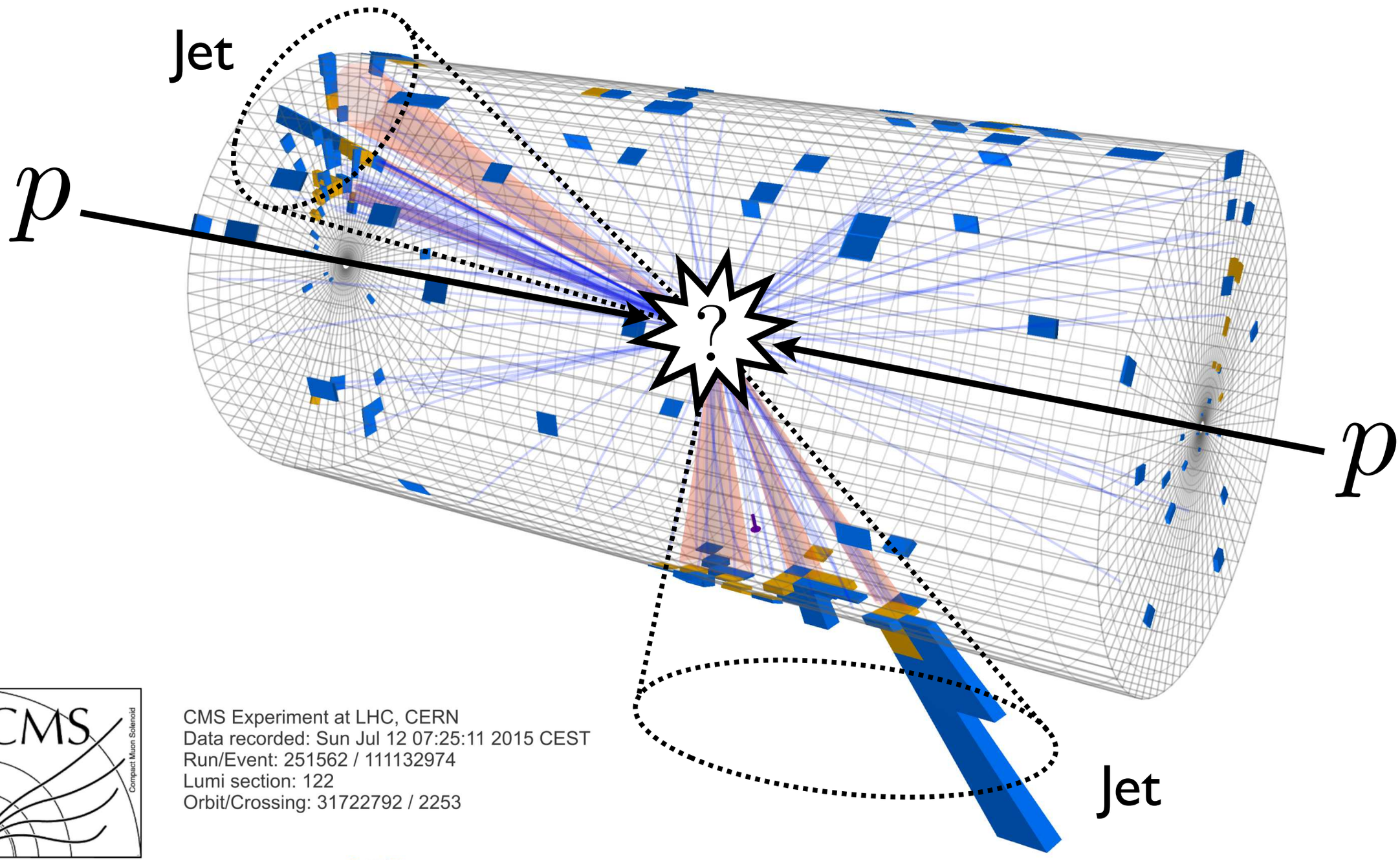
University of Maryland Physics Colloquium — October 13, 2020

# Wearing my New Hat…

**The NSF AI Institute for**
**Artificial Intelligence and Fundamental Interactions**

*Postdoctoral fellowship opportunity (Oct 20 deadline):*
*http://iaifi.org/fellows.html*

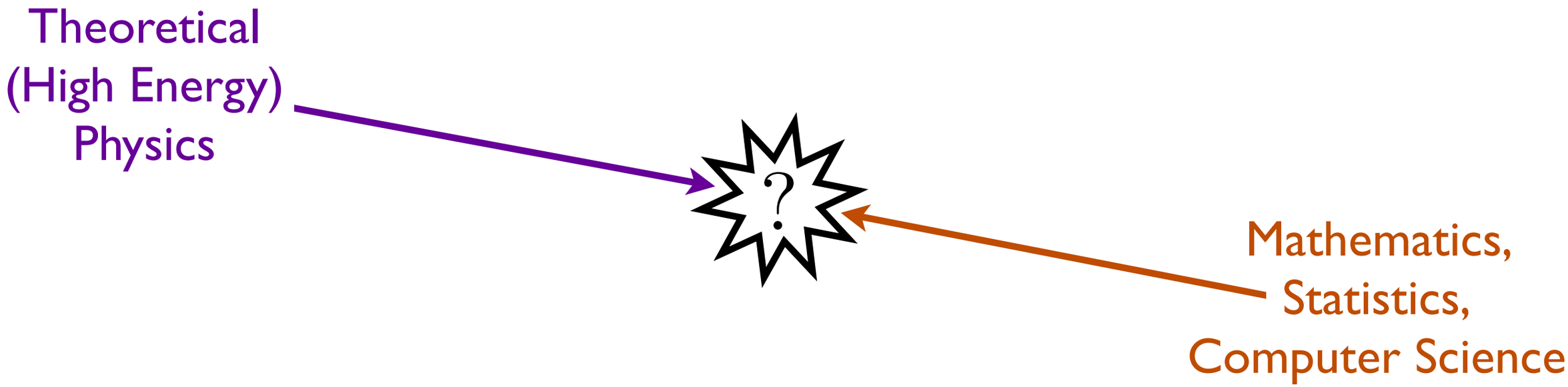
# “Collision Course”




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

# “Collision Course”

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



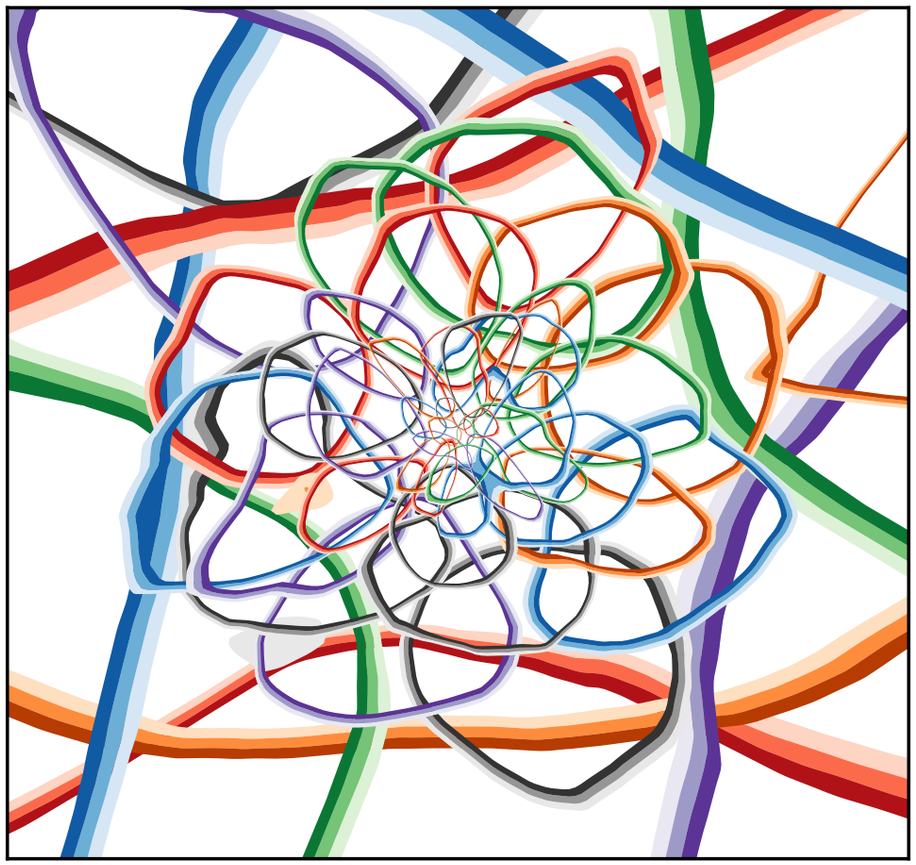

*New insights into particle physics**
*facilitated by advances in machine learning**

*(and vice versa?)*

# Today's Talk: Two Anecdotes

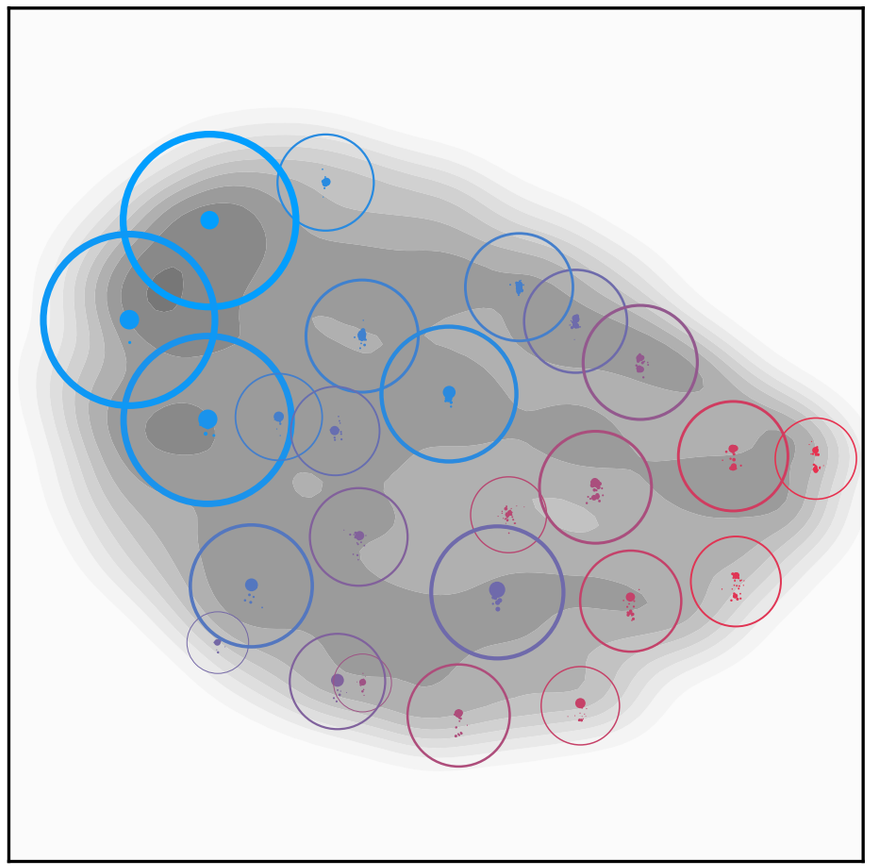



## Teaching a Machine to "Think Like a Physicist"



[Komiske, Metodiev, JDT, JHEP 2019]

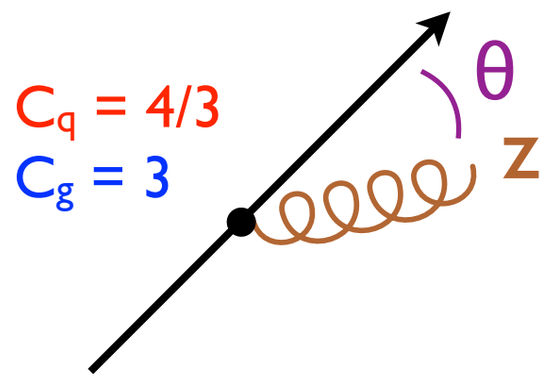
## Letting Collider Data Speak for Itself



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

*Data analysis strategies motivated by the symmetries and structures of particle physics*

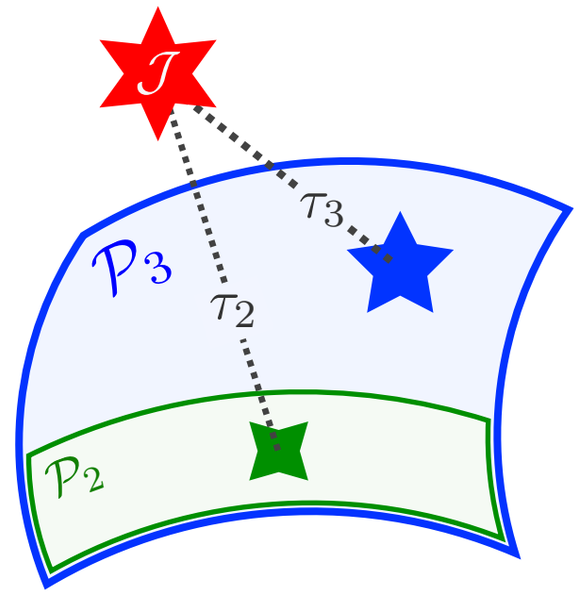
## Exploiting a Core Prediction of QCD




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

[Altarelli, Parisi, NPB 1977]

## Nested Singularities of Gauge Theories

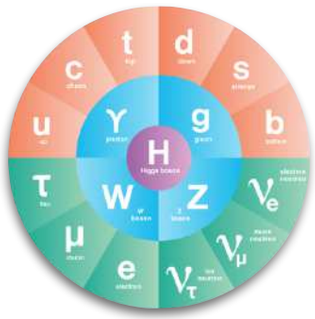



$$\tau_N(\mathcal{J}) = \min_{\mathcal{J}' \in \mathcal{P}_N} \mathrm{EMD}(\mathcal{J}, \mathcal{J}')$$

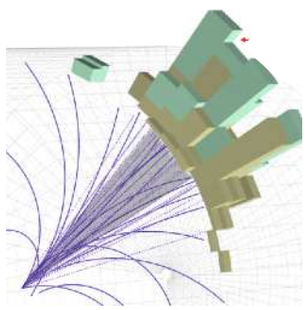
[Stewart, Tackmann, Waalewijn, PRL 2010; JDT, Van Tilburg, JHEP 2011, JHEP 2012; rephrased via Komiske, Metodiev, JDT, JHEP 2020]

*New perspectives on key theoretical concepts*

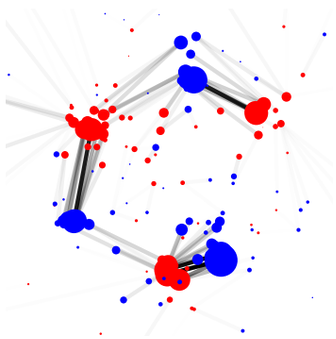
# Outline



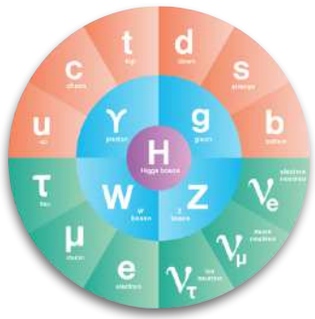

## Particle Physics 101



## What is a Collider Event?



## When are Collider Events Similar?




# Particle Physics 101



## What is a Collider Event?

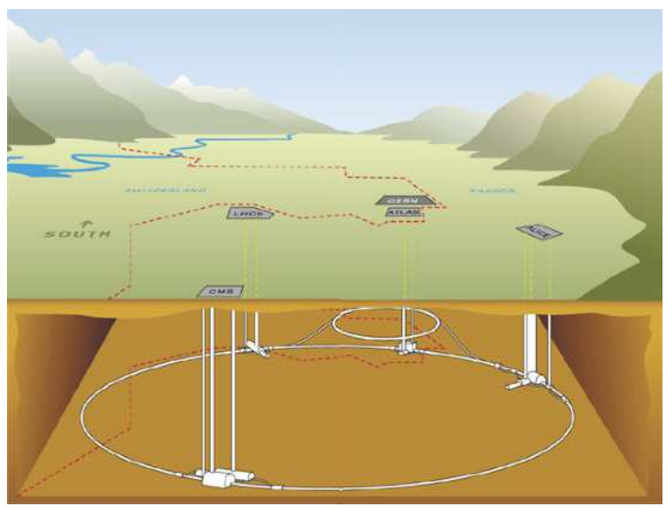


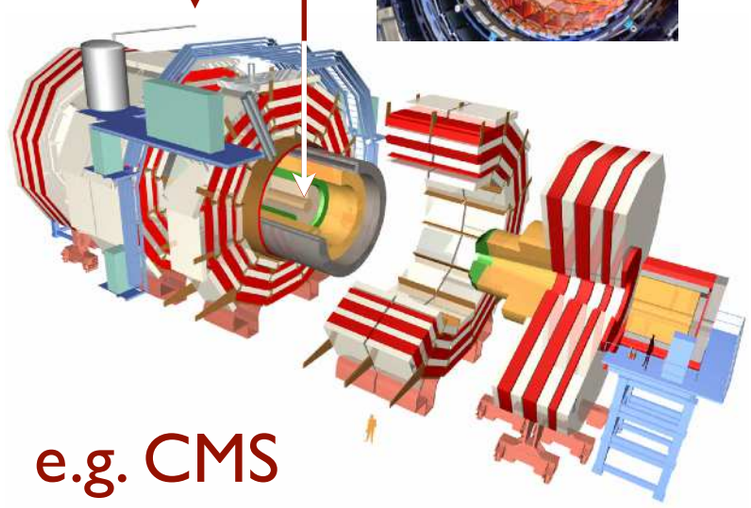
## When are Collider Events Similar?

The Universe
Galaxy
Solar System
Planet
Us
Hairs
Cells
Molecules
Electrons
Protons
The TeV Scale
Grand Unification
Quantum Gravity

$10^{26}$ m $10^{11}$ m $10^{-4}$ m $10^{-19}$ m $10^{-34}$ m

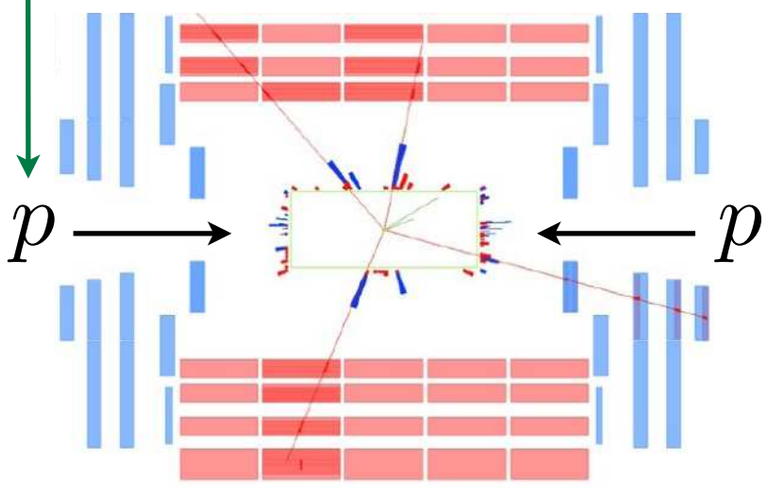
LHC



e.g. CMS

E = hc/λ



## Mesons

$$\pi^{\pm}\,\pi^{0}\,\eta\,K^{\pm}\,K^{0}\,\eta'\,D^{\pm}\,D^{0}\,D_s^{\pm}\,\eta_c\,B^{\pm}\,B^{0}\,B_s^{0}\,\eta_b\,\ldots$$

$$\rho^{\pm}\,\rho^{0}\,\omega\,K^{*\pm}\,K^{*0}\,\phi\,D^{*\pm}\,D^{*0}\,D_s^{*\pm}\,J/\psi\,B^{*\pm}\,B^{*0}\,B_s^{*0}\,\Upsilon\,\ldots$$

## Baryons

$$p\,n\,\Lambda^{0}\,\Sigma^{+}\,\Sigma^{0}\,\Sigma^{-}\,\Xi^{0}\,\Xi^{-}\,\ldots$$

$$\Delta^{++}\,\Delta^{+}\,\Delta^{0}\,\Delta^{-}\,\Sigma^{*+}\,\Sigma^{*0}\,\Sigma^{*-}\,\Xi^{*0}\,\Xi^{*-}\,\Omega^{-}\,\ldots$$

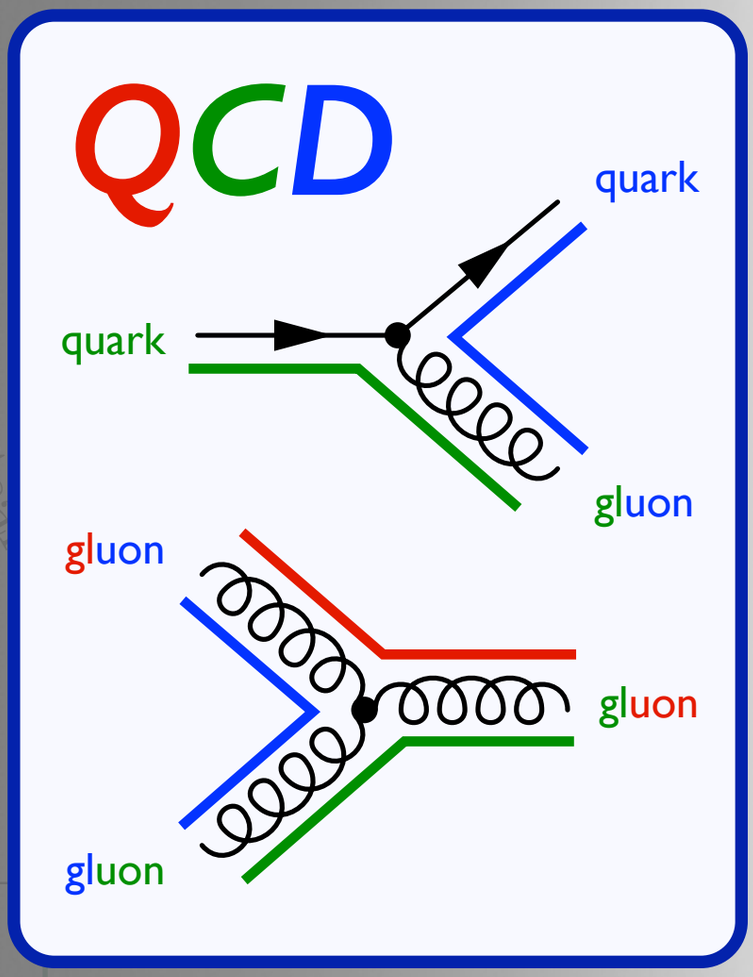
## Tetraquarks

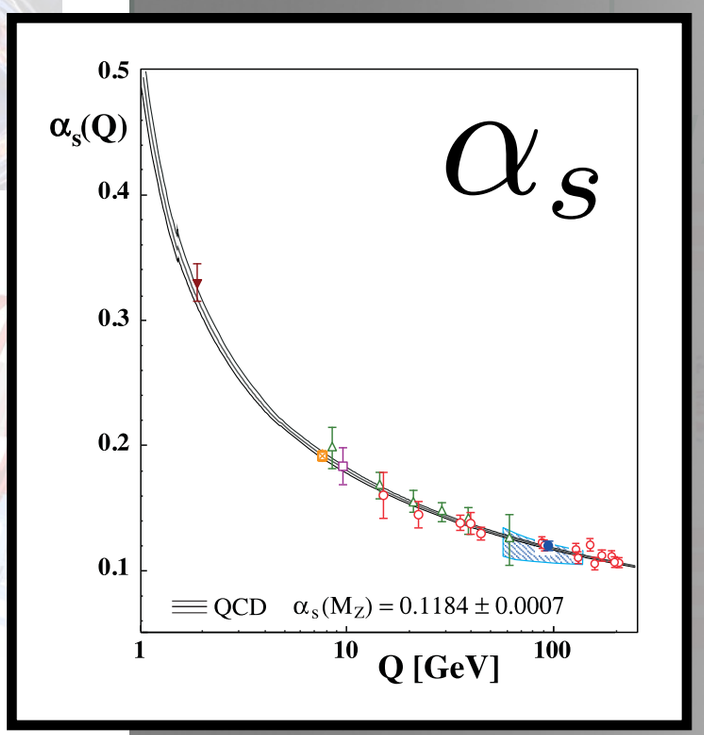
$$X(3872)\,Y(4260)\,Z(4430)\,\ldots$$

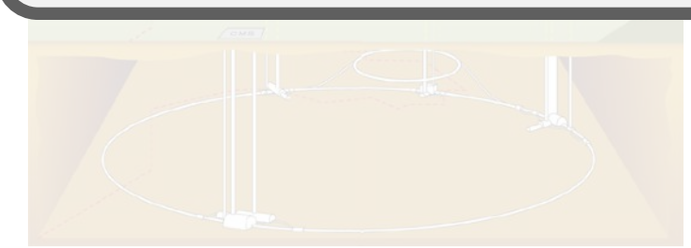
## Pentaquarks

$$P_c^{+}(4450)\,\ldots$$

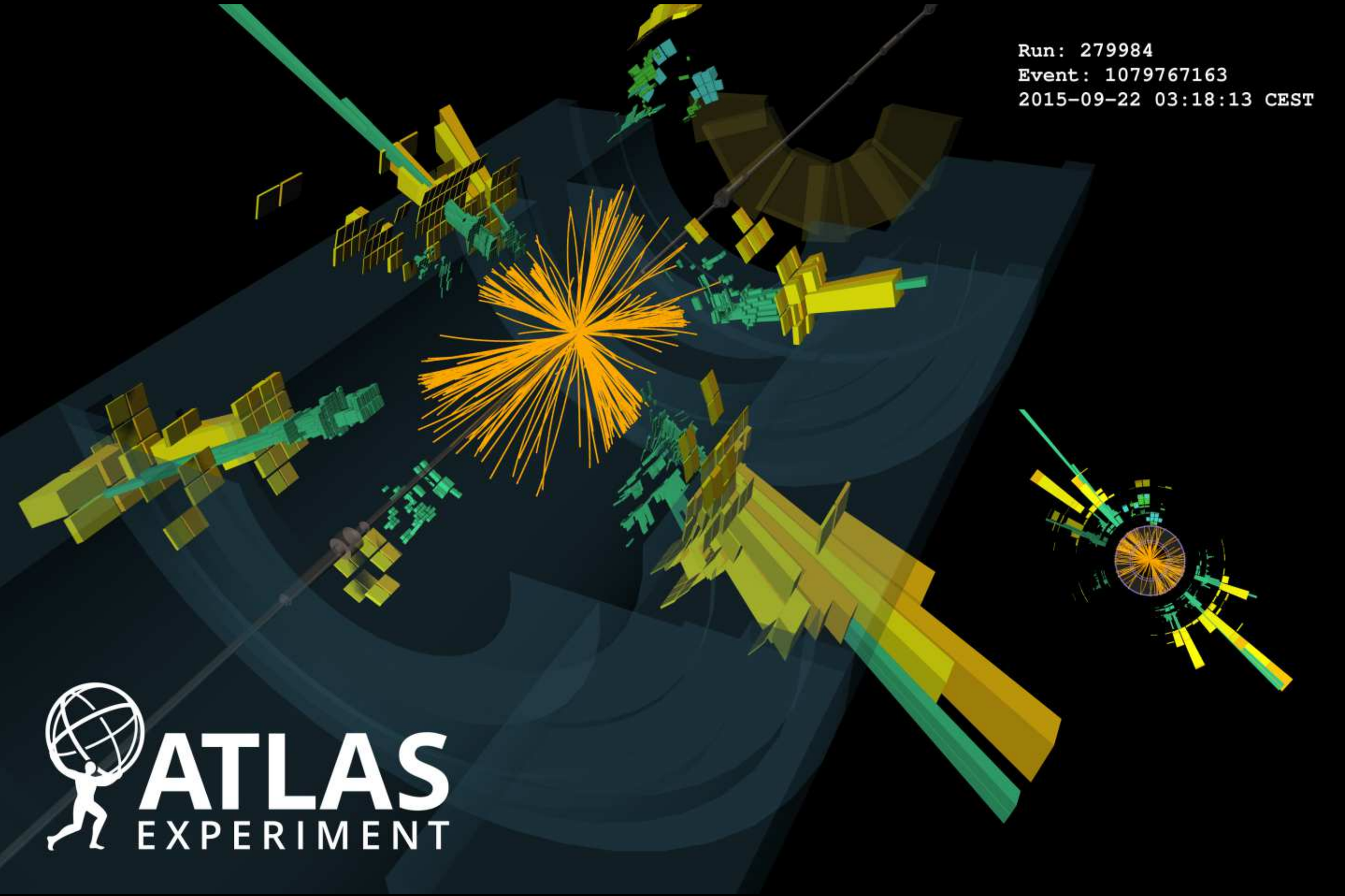
Jets



e.g. CMS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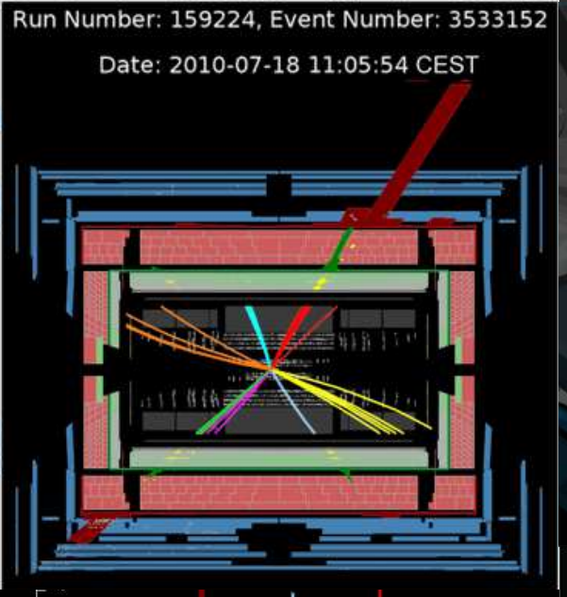
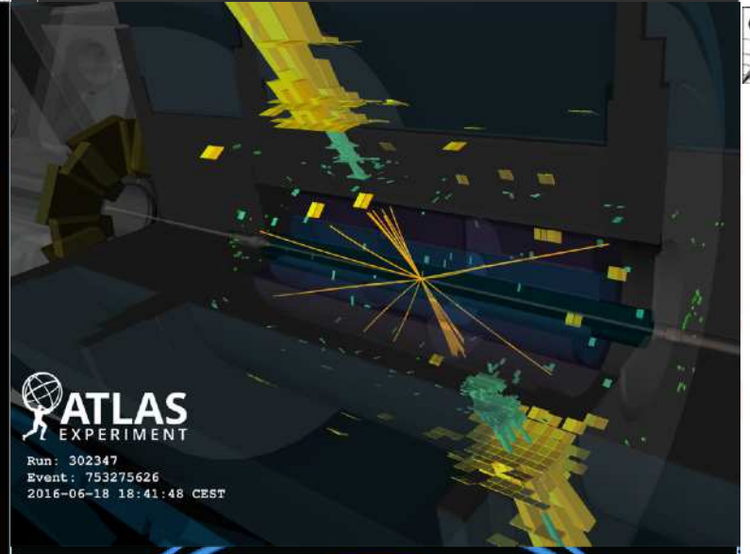
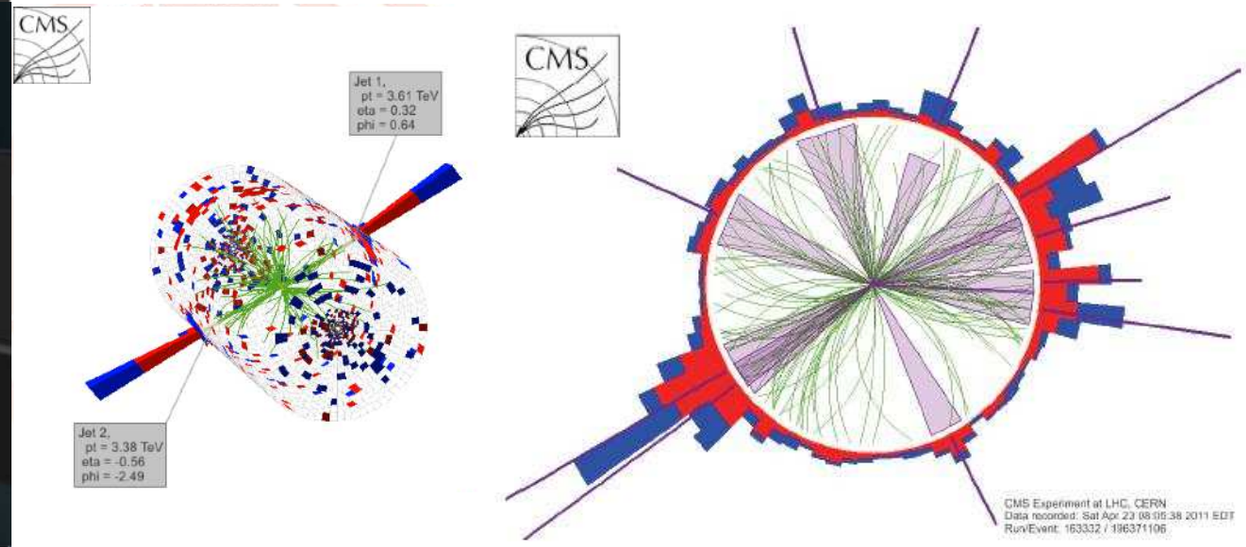
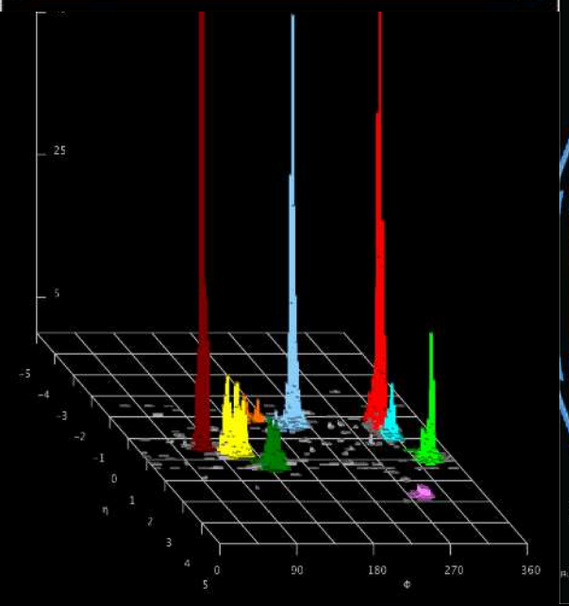
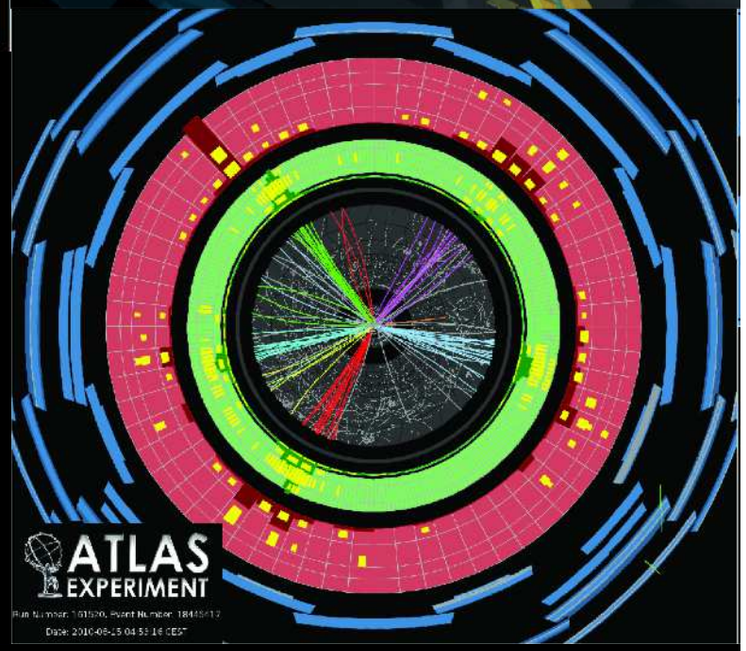
Event: 1079767163
2015-09-22 03:18:13 CEST
ATLAS
EXPERIMENT

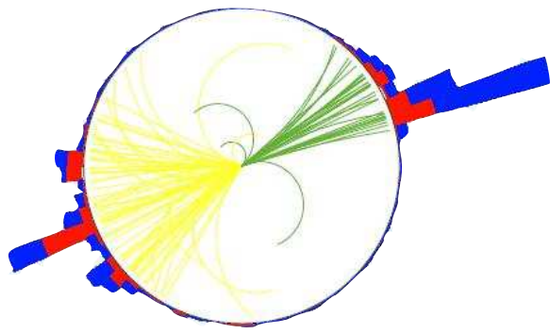

Run Number: 159224, Event Number: 3533152
Date: 2010-07-18 11:05:54 CEST

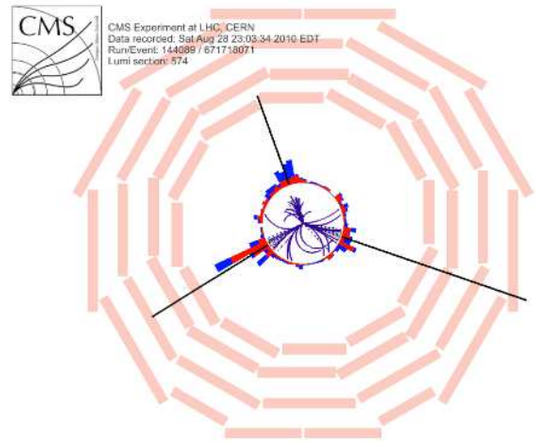

ATLAS
EXPERIMENT
Run: 302347
Event: 753275626
2016-06-18 18:41:48 CEST

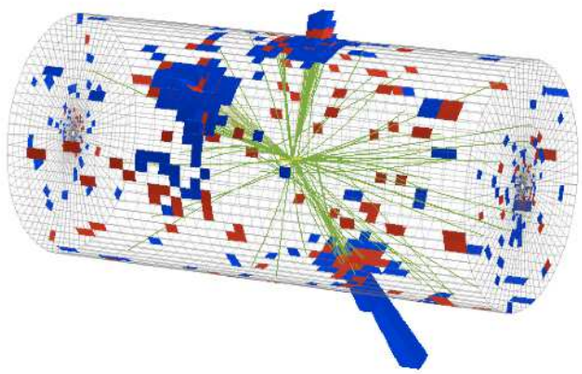

CMS
Jet 1,
pt = 3.61 TeV
eta = 0.32
phi = 0.64
Jet 2,
pt = 3.38 TeV
eta = -0.56
phi = -2.49
CMS
CMS Experiment at LHC, CERN
Data recorded: Sat Apr 23 08:05:38 2011 EDT
Run/Event: 163332 / 196371106

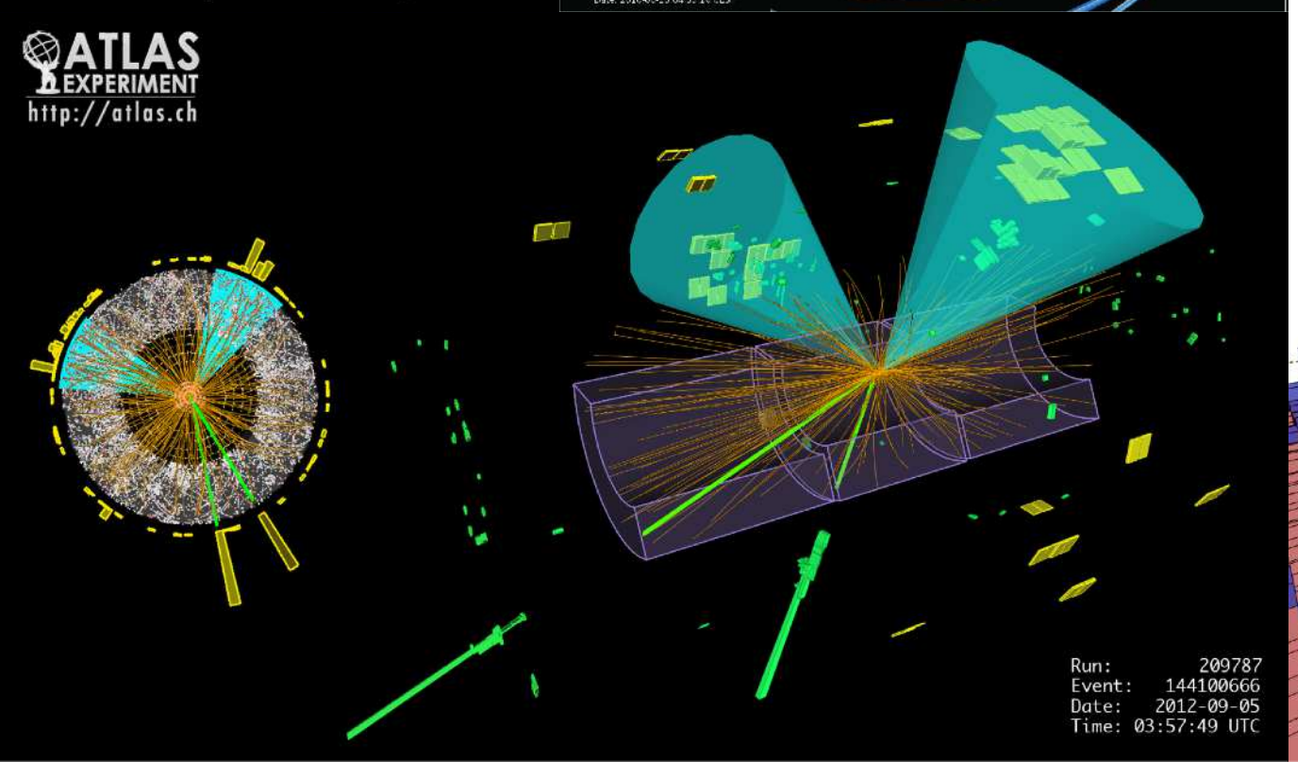

25
5
-5
-4
-3
-2
-1
0
1
2
3
4
5
0
90
180
270
360
η
φ

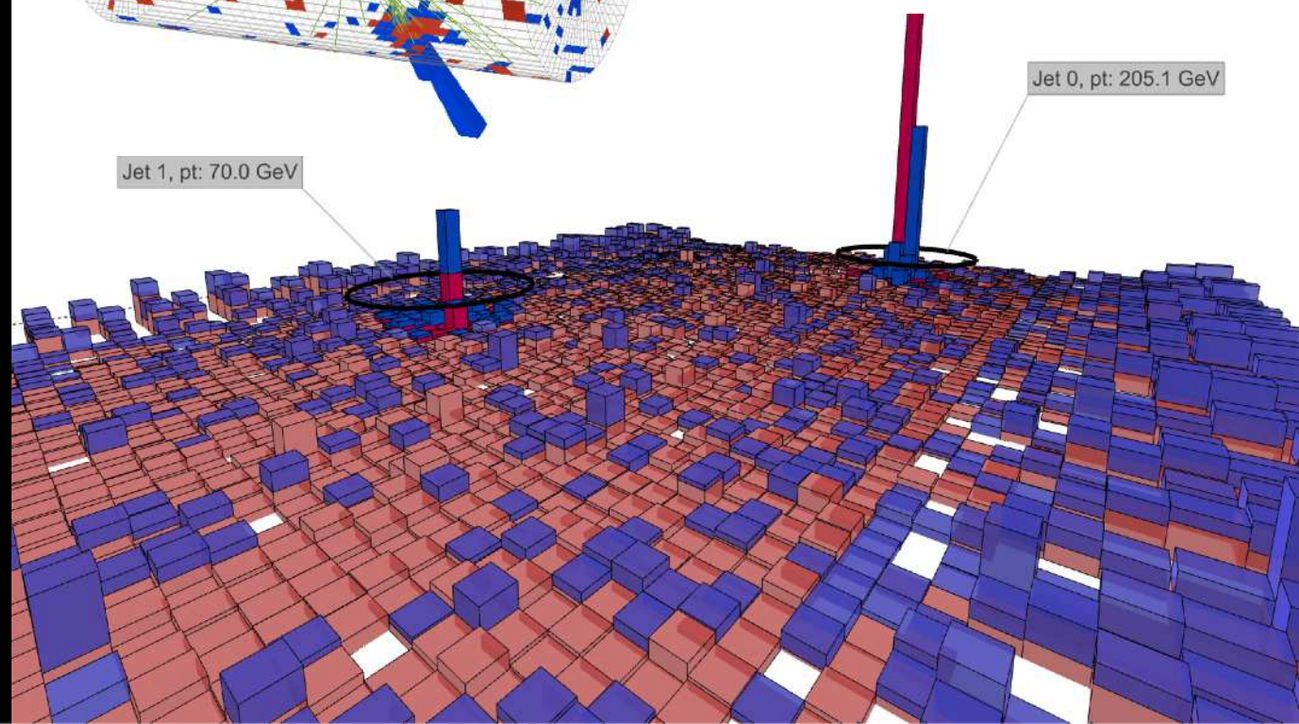

ATLAS
EXPERIMENT

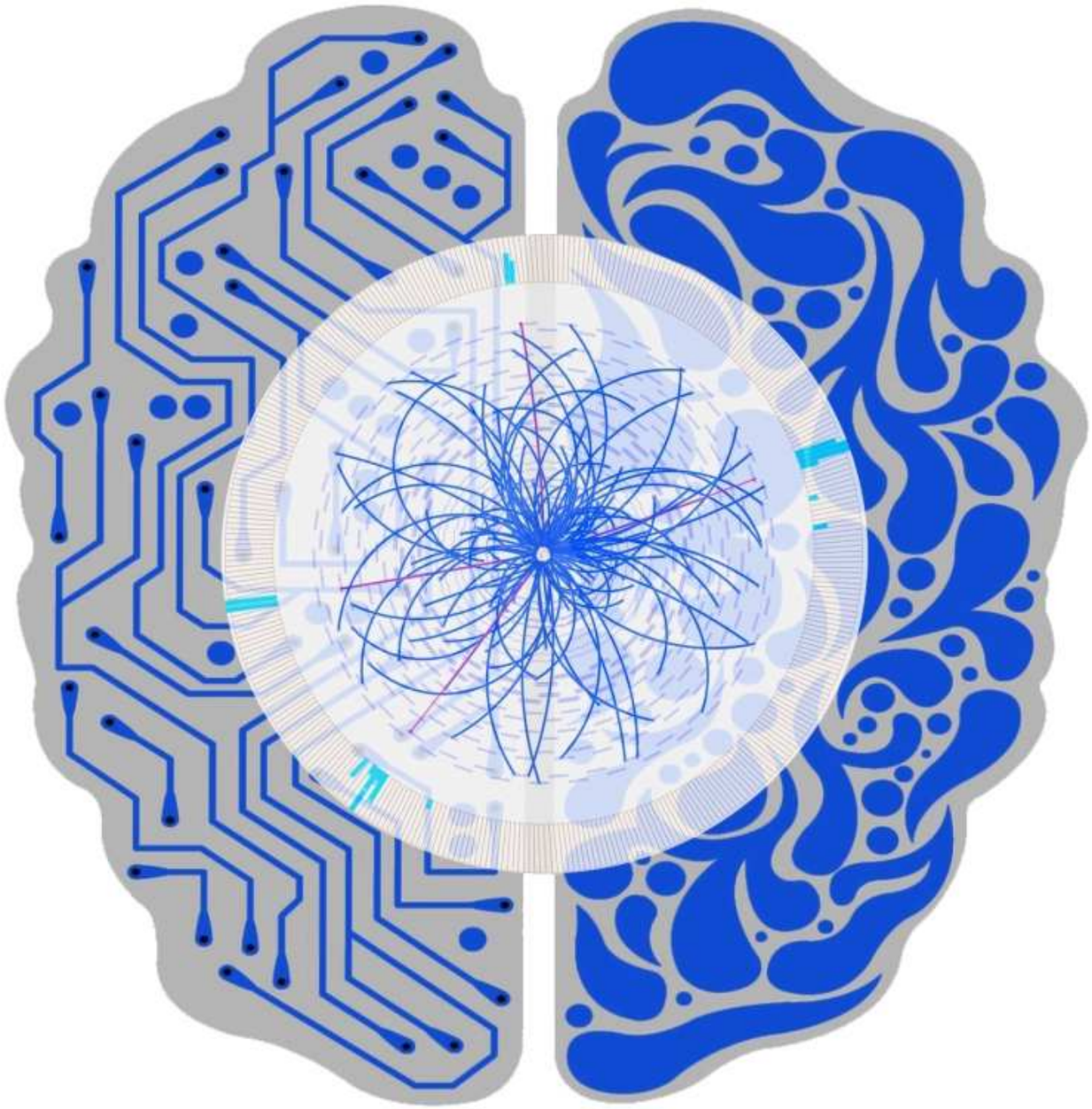



CMS
CMS Experiment at LHC, CERN
Data recorded: Sat Aug 28 23:03:34 2010 EDT
Run/Event: 144089 / 671718071
Lumi section: 574




ATLAS
EXPERIMENT
http://atlas.ch
Run: 209787
Event: 144100666
Date: 2012-09-05
Time: 03:57:49 UTC

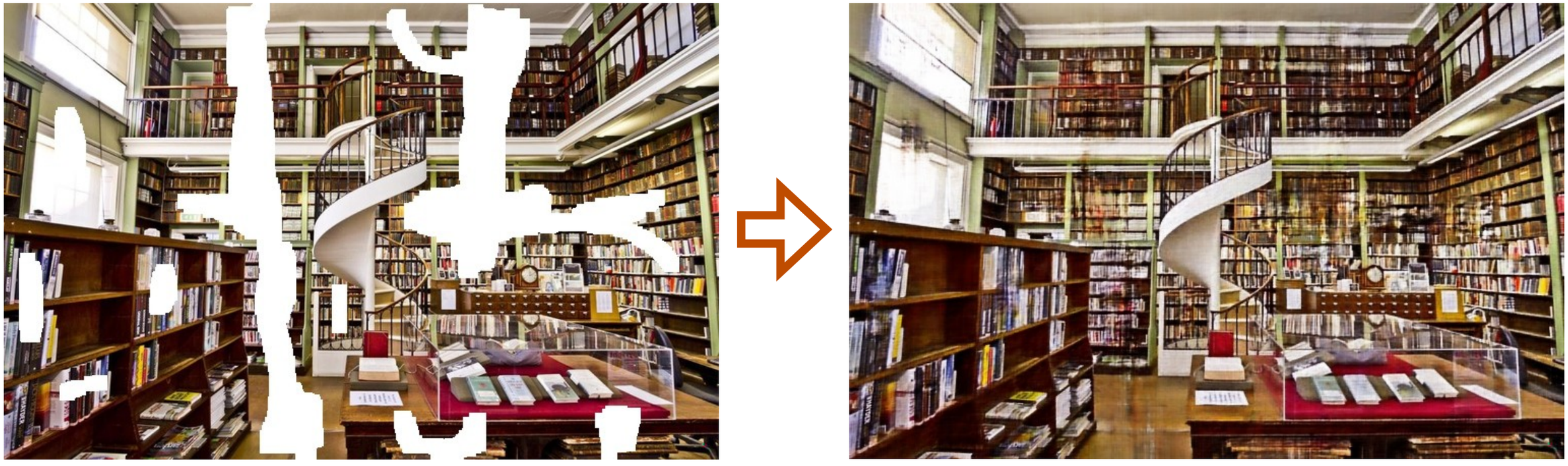

Jet 0, pt: 205.1 GeV
Jet 1, pt: 70.0 GeV



# *The Rise of Machine Learning*

# Deep Learning

*E.g. Inpainting*

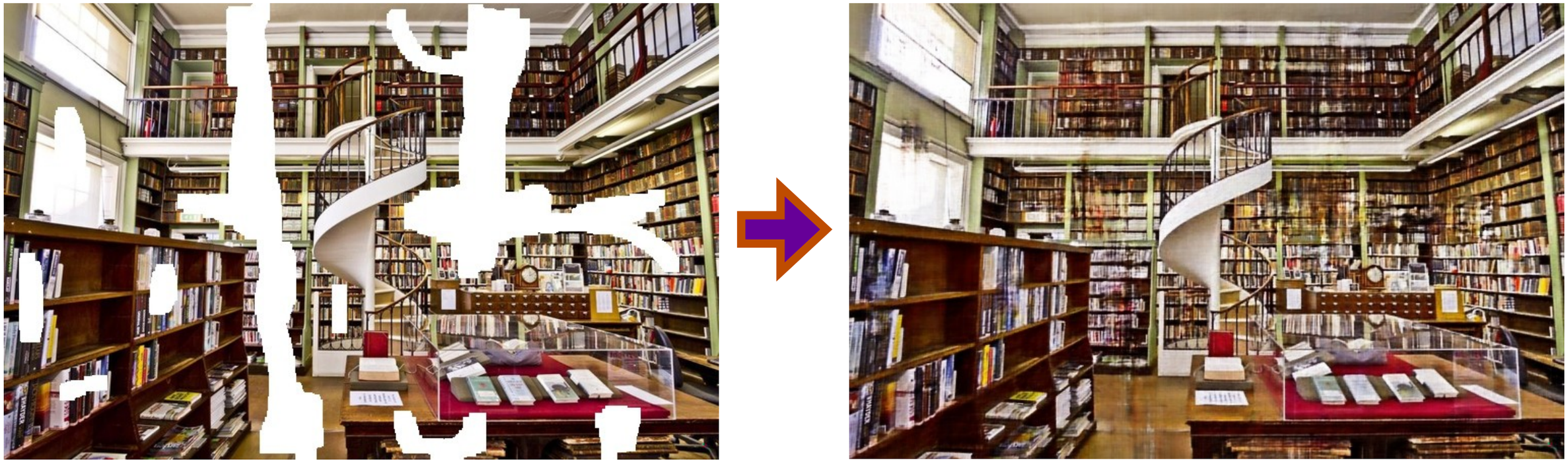


increased computational power and large data sets

[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

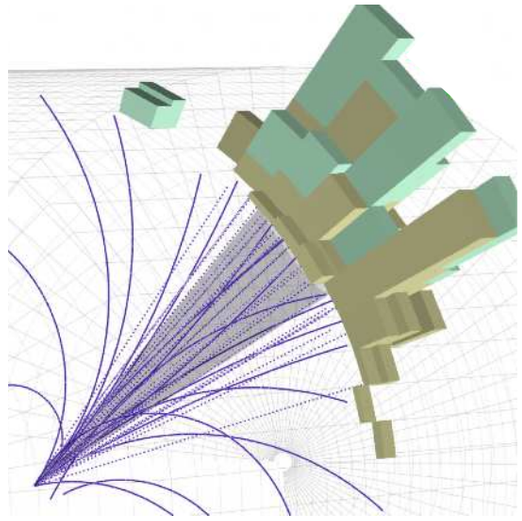
(not just increased computational power and large data sets)

[Ulyanov, Vedaldi, Lempitsky, CVPR 2018]

# Cartoon of Machine Learning

*"ML4Jets"*
*NYU, January 2020*

For this talk: $\mathcal{J}$ = jet



Properly specified problem

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

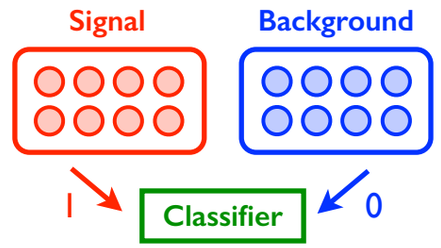
The Machine

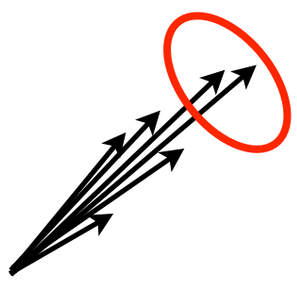
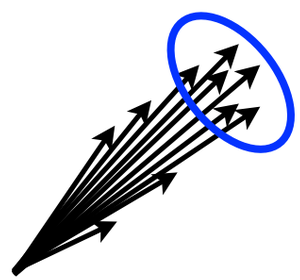
Solution $S(\mathcal{J})$

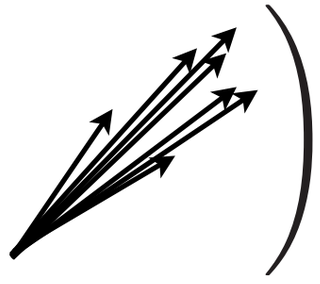
E.g.: Problem = Minimize loss function
Solution = Multi-layer neural network
Strategy = Stochastic gradient descent

# Quark/Gluon Classification

*"Hello, World!" of Jet Physics*




e.g.  **Quark** $C_q = 4/3$ vs.  **Gluon** $C_g = 3 = 9/3$

Find $h\left(\right.$  $\left.\right)$ such that $h\left(\text{Quark}\right) = 1$, $h\left(\text{Gluon}\right) = 0$

Best you can do: $h(\mathcal{J}) = \dfrac{p(\mathcal{J}|\mathrm{Q})}{p(\mathcal{J}|\mathrm{Q}) + p(\mathcal{J}|\mathrm{G})}$

(Neyman-Pearson lemma)

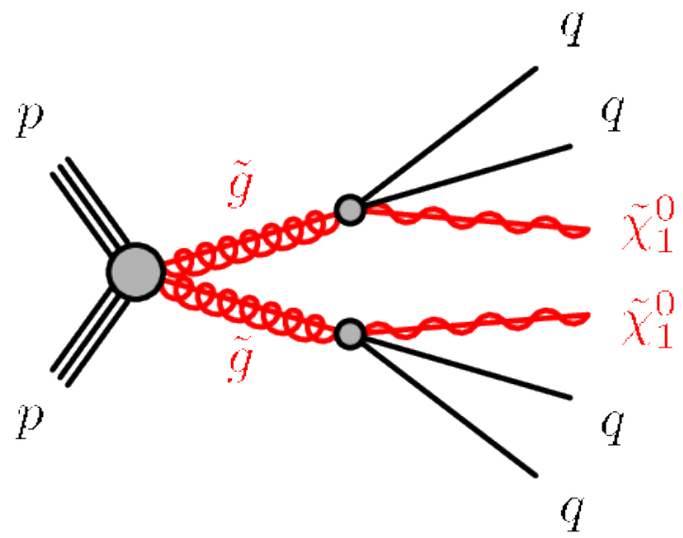
# E.g. Search for Supersymmetry


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

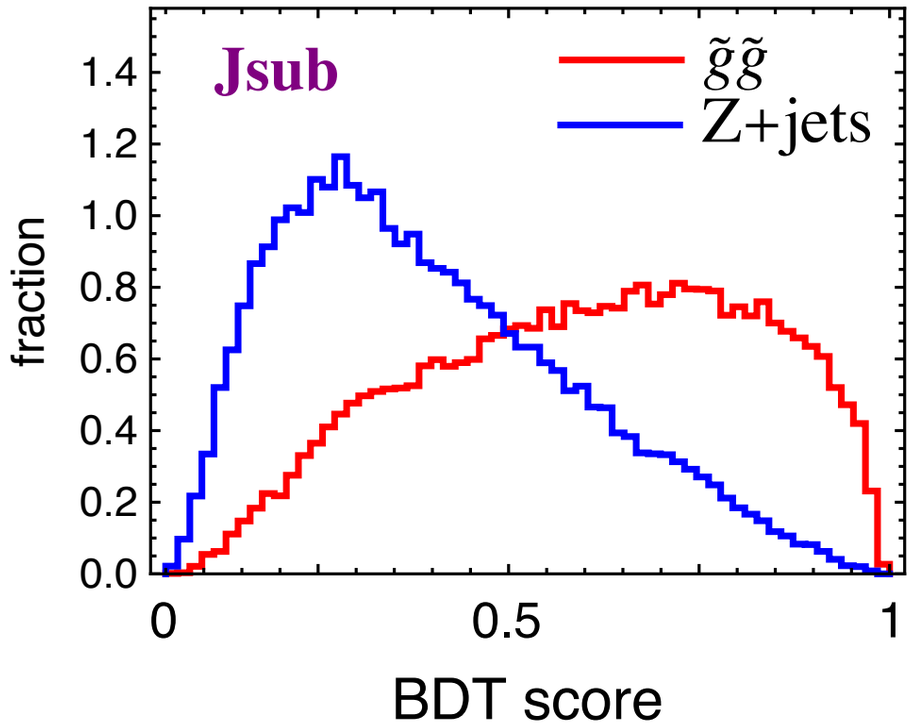
Inputs: Jet mass, width, track multiplicity

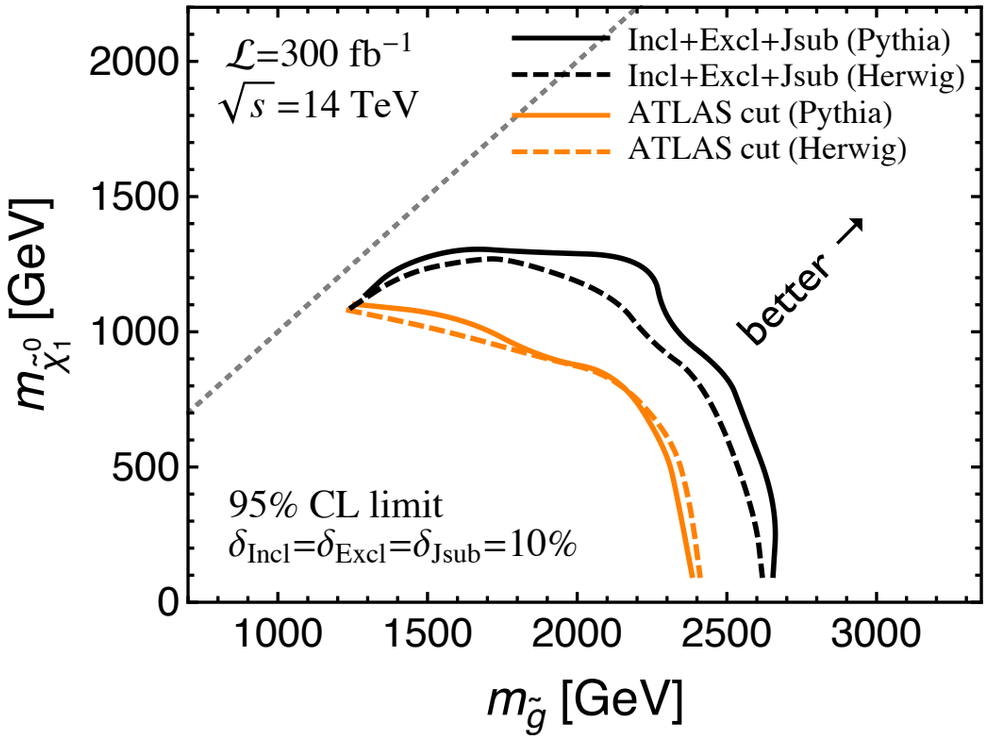
Signal: **Quark enriched**

Background: **Gluon enriched**



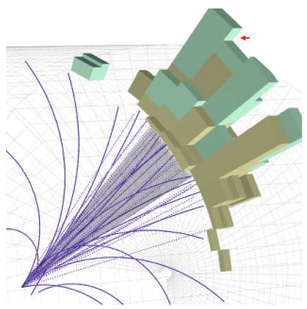

← background signal →




[Bhattacherjee, Mukhopadhyay, Nojiri, Sakakie, Webber, JHEP 2017]

# Particle Physics 101



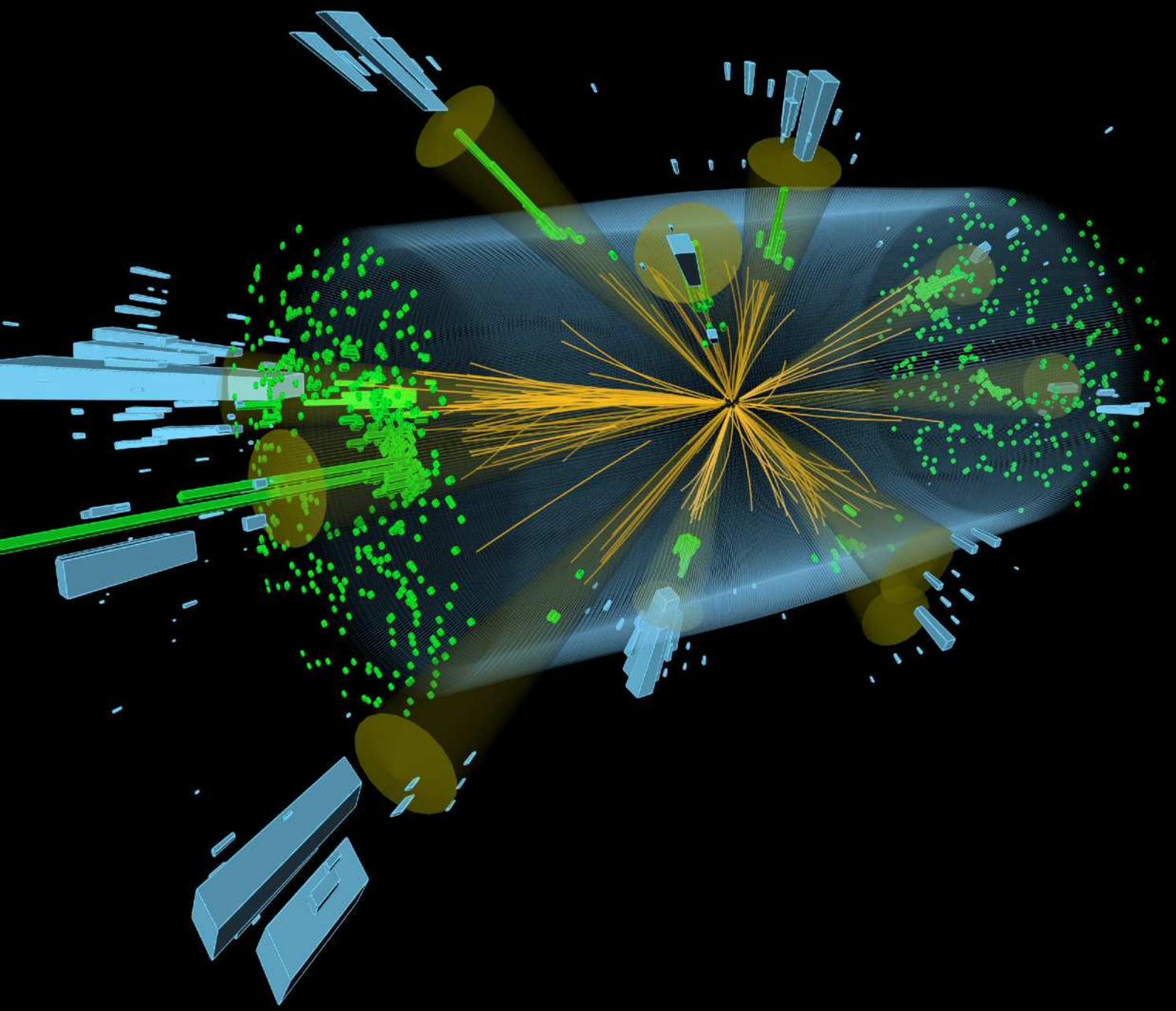
## What is a Collider Event?



## When are Collider Events Similar?

# *Collider Event*

Collection of points in (momentum) space

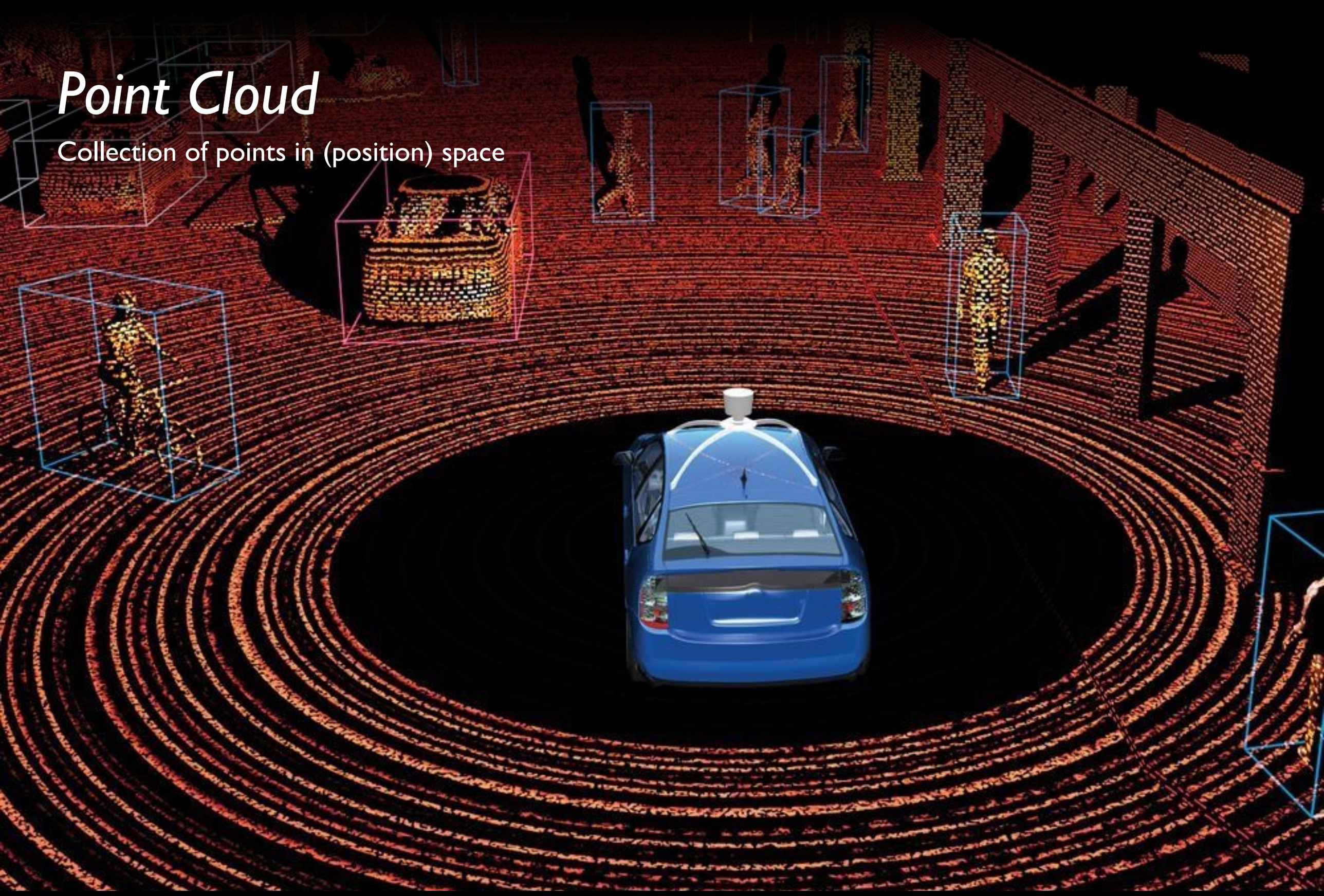


T E H M

| | | |
|---|---|---|
| $\gamma$ | photon | elementary |
| $e^{\pm}$ | electron | elementary |
| $\mu^{\pm}$ | muon | elementary |
| $\pi^{\pm}$ | pion | composite |
| $K^{\pm}$ | kaon | composite |
| $K^0_L$ | K-long | composite |
| $p/\overline{p}$ | proton | composite |
| $n/\overline{n}$ | neutron | composite |

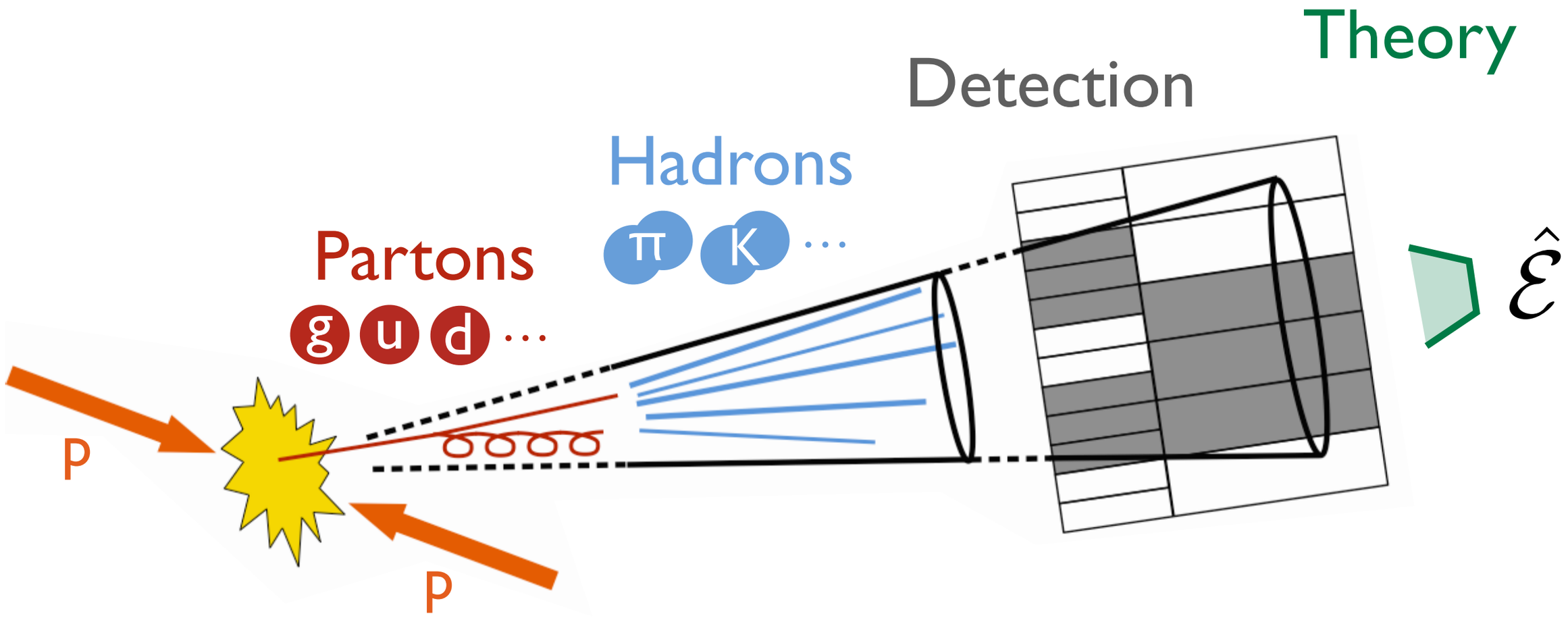
# *Point Cloud*

Collection of points in (position) space



[Popular Science, 2013]

# Dynamics of Jet Formation




## *Energy Flow:*

Robust to hadronization and detector effects

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

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

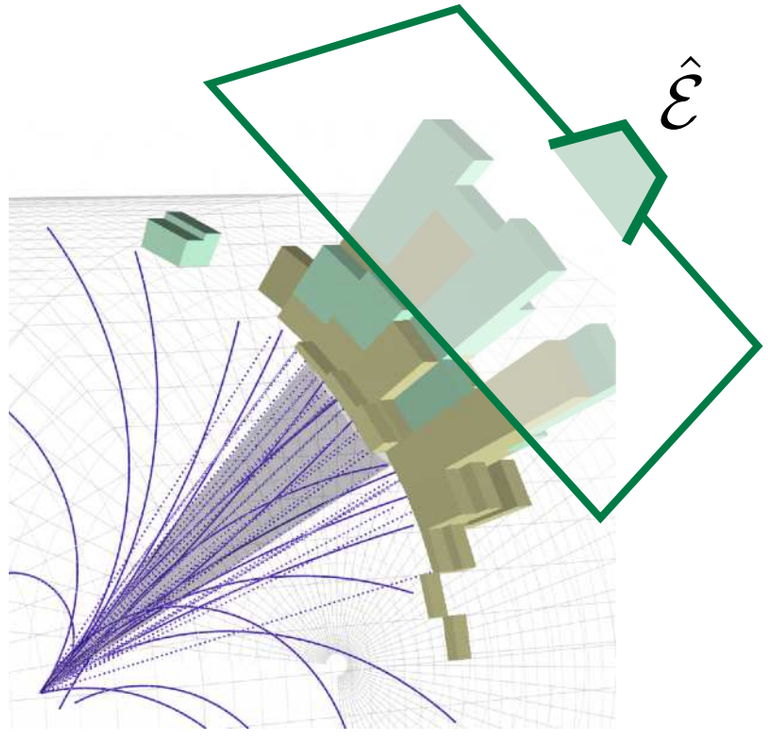
# Jets as Weighted Point Clouds

- Energy-Weighted Directions

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

Energy — Direction

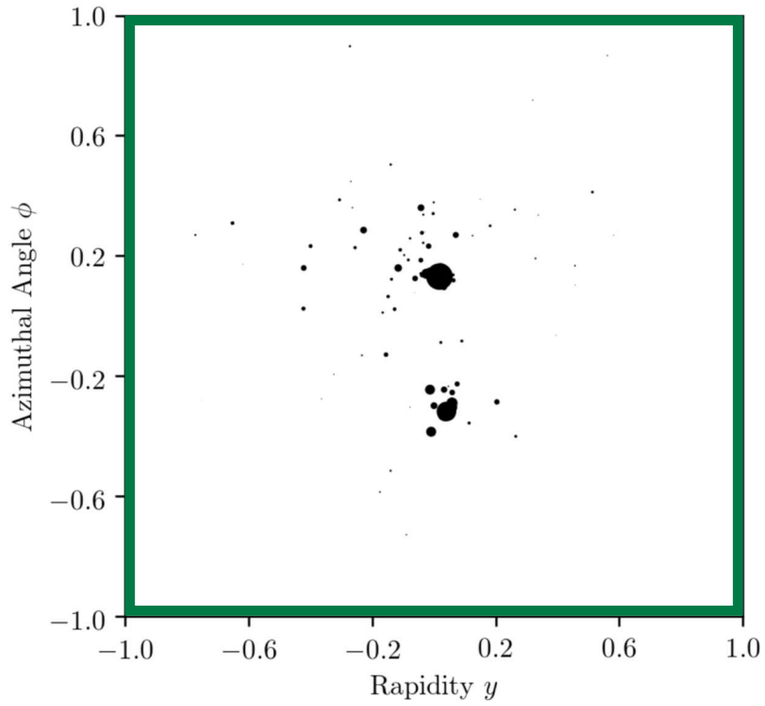
(suppressing "unsafe" charge/flavor information)




- Equivalently: Energy Density

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

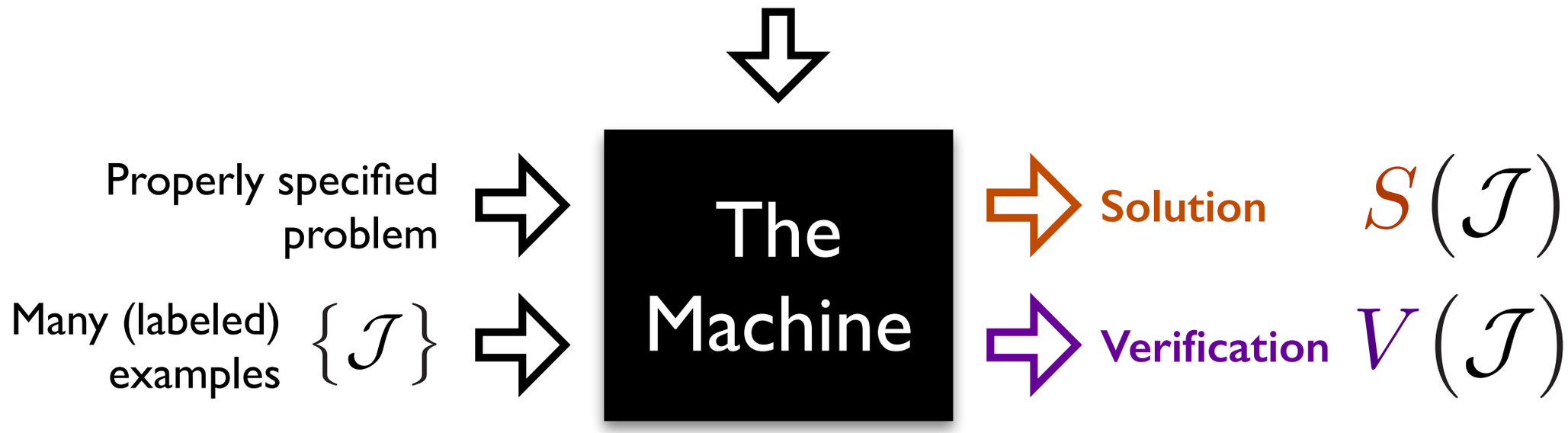
Energy — Direction



# "Thinking" Like a Physicist

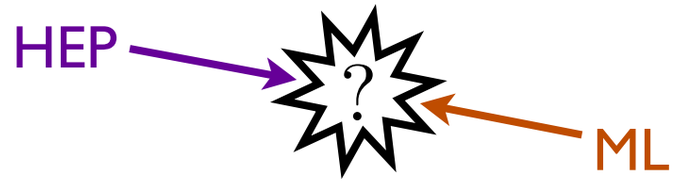
**Symmetry:** $\mathcal{J} = \{\underbrace{\vec{p}_1, \vec{p}_2, \vec{p}_3, \ldots, \vec{p}_N}_{\text{Unordered, Variable Length Set (QM!)}}\}$

**Safety:** $\vec{p} = \{\underbrace{E}_{\text{Energy weighting (QFT!)}}, \hat{n}_x, \hat{n}_y, \hat{n}_z\}$




*Check that answer is physically sensible*

# Energy Flow Networks




*Architecture designed around symmetries and interpretability*

Permutation invariant

Linear weights (i.e. safe)

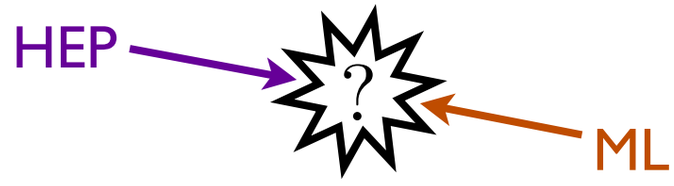
$$S(\mathcal{J}) = F\big(V_1, V_2, \ldots, V_\ell\big) \qquad V_a(\mathcal{J}) = \sum_{i\in\mathcal{J}} E_i\, \Phi_a(\hat{n}_i)$$

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



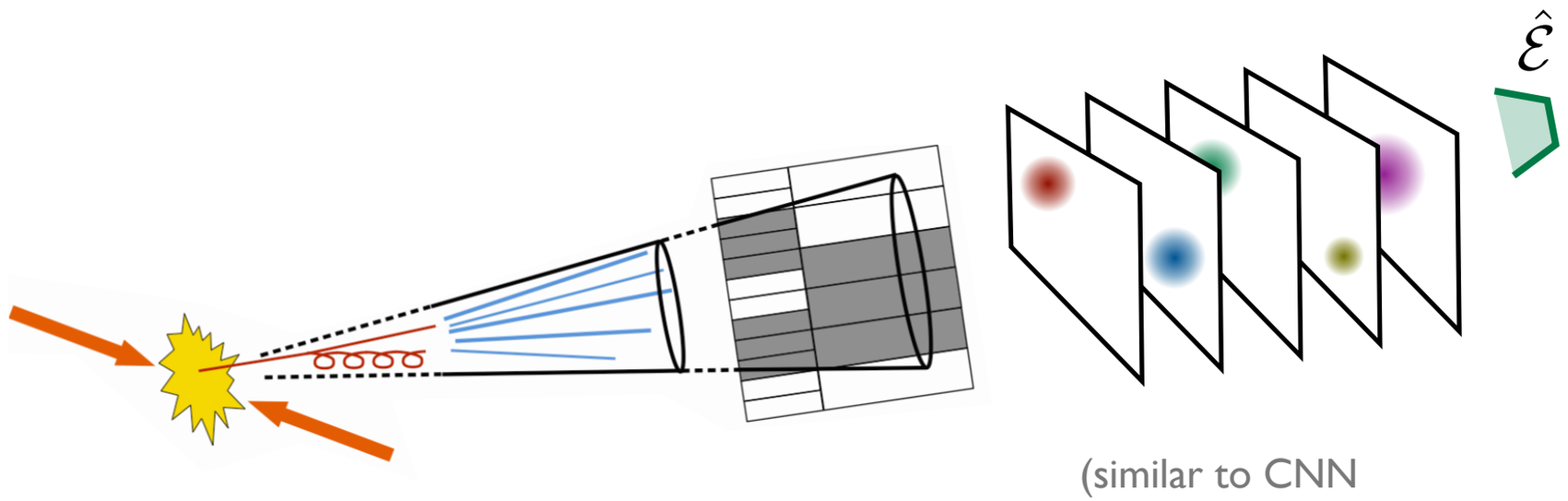

*Architecture designed around symmetries and **interpretability***

Latent space of dim $\ell$

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

Can visualize if $\ell$ is small

Easy to plot!

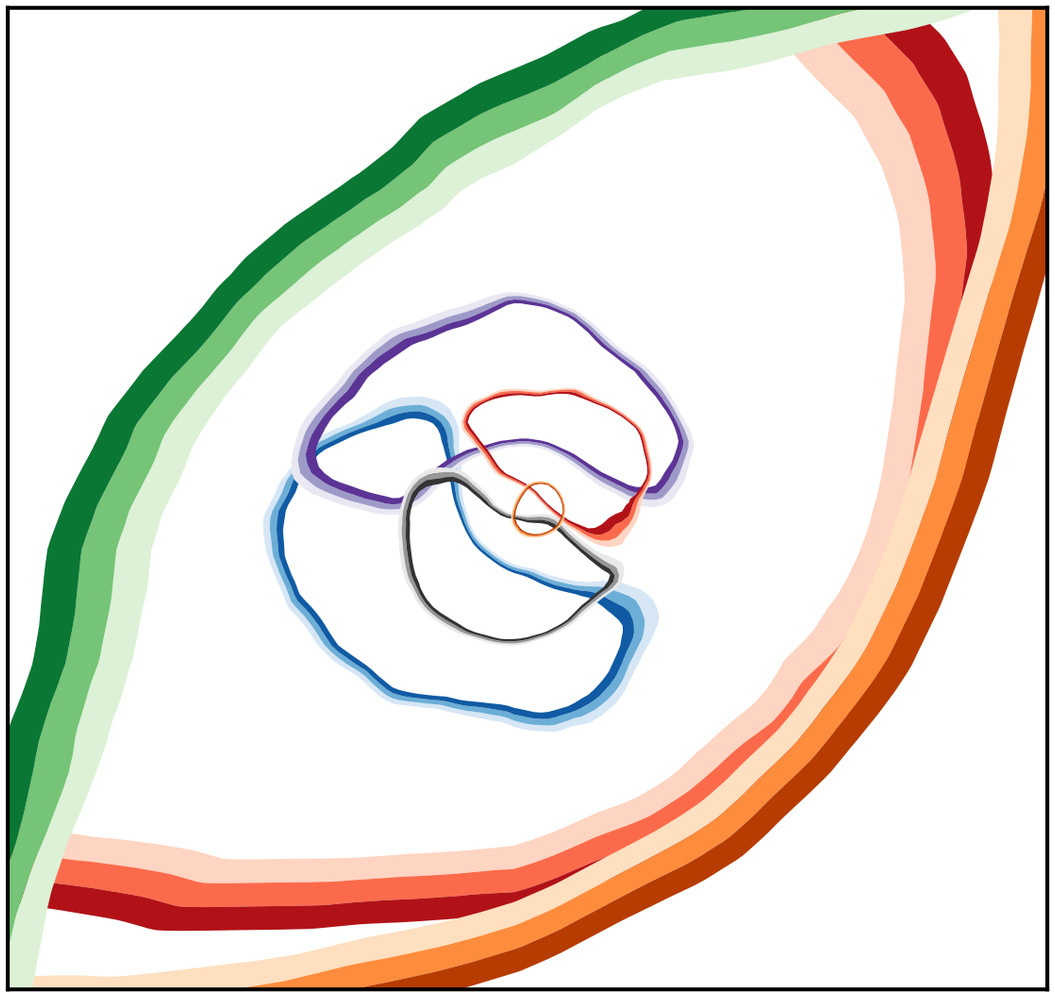



(similar to CNN filter activation)

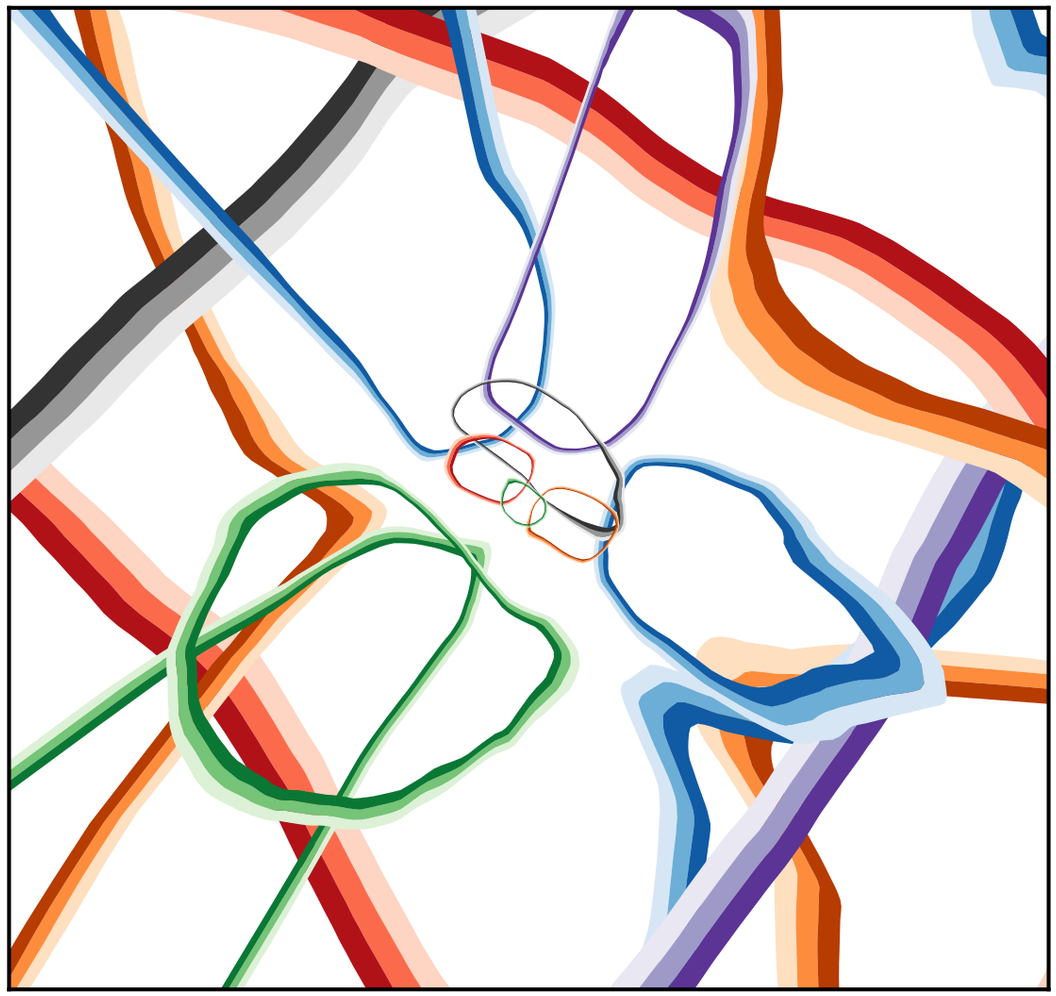
[Komiske, Metodiev, JDT, JHEP 2019; see also Komiske, Metodiev, JDT, JHEP 2018; code at energyflow.network; special case of Zaheer, Kottur, Ravanbakhsh, Poczos, Salakhutdinov, Smola, NIPS 2017]


# Psychedelic Network Visualization

Latent Dimension 8



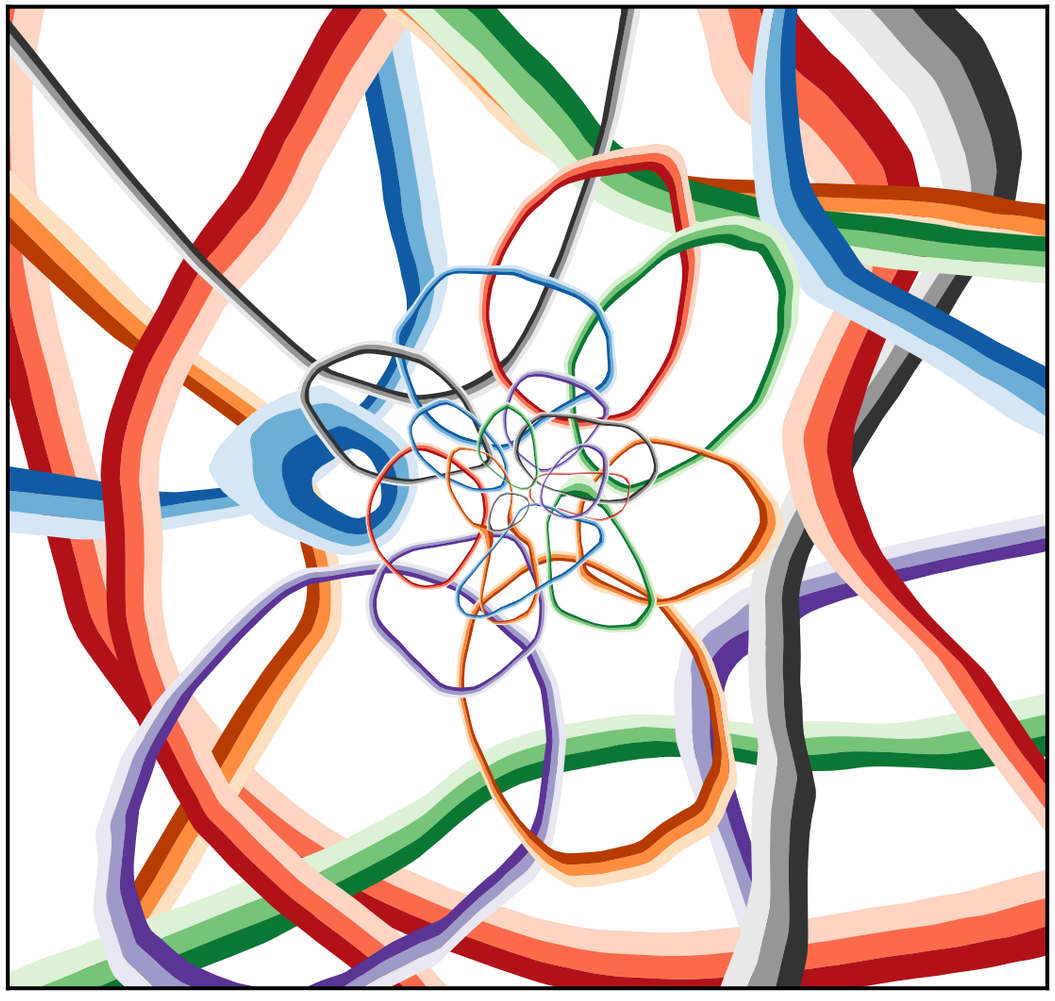
Latent Dimension 16



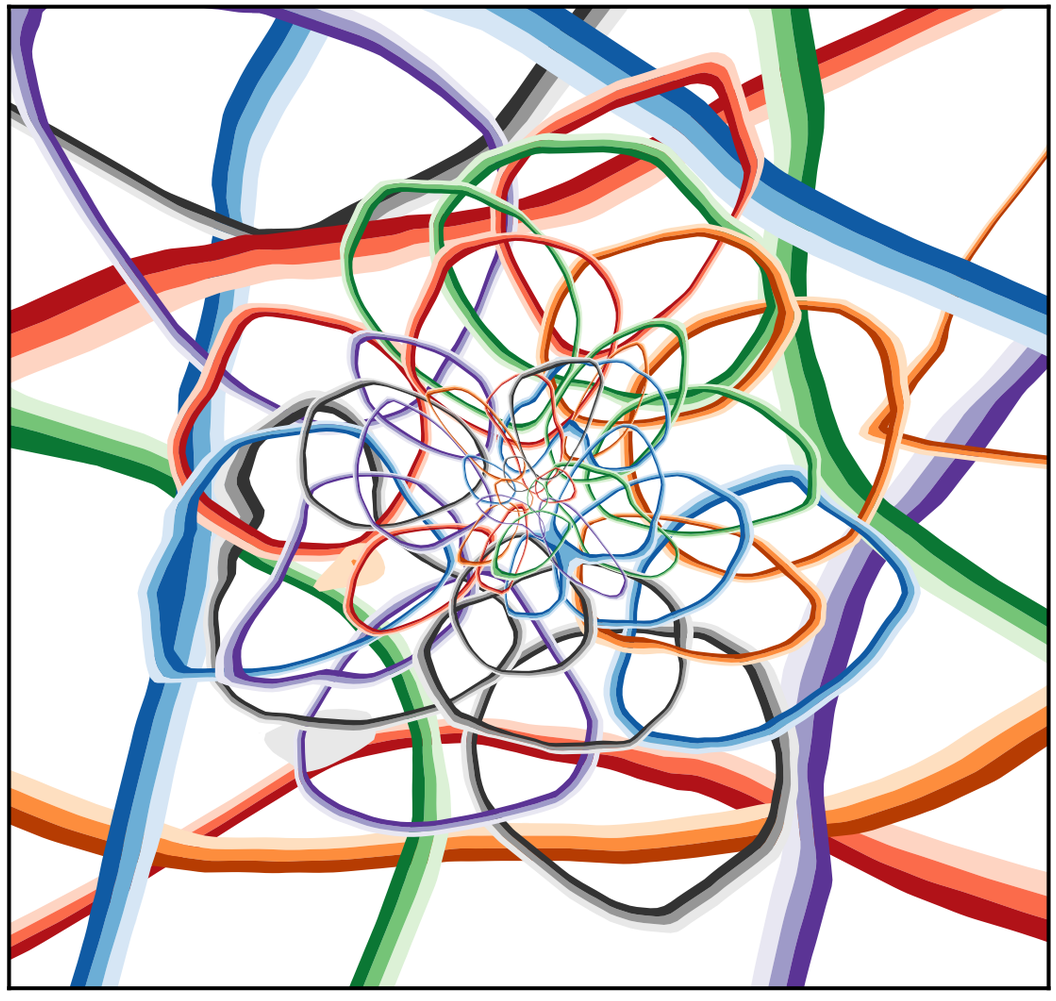
For the case of quark vs. gluon classification

# Psychedelic Network Visualization

Latent Dimension 32

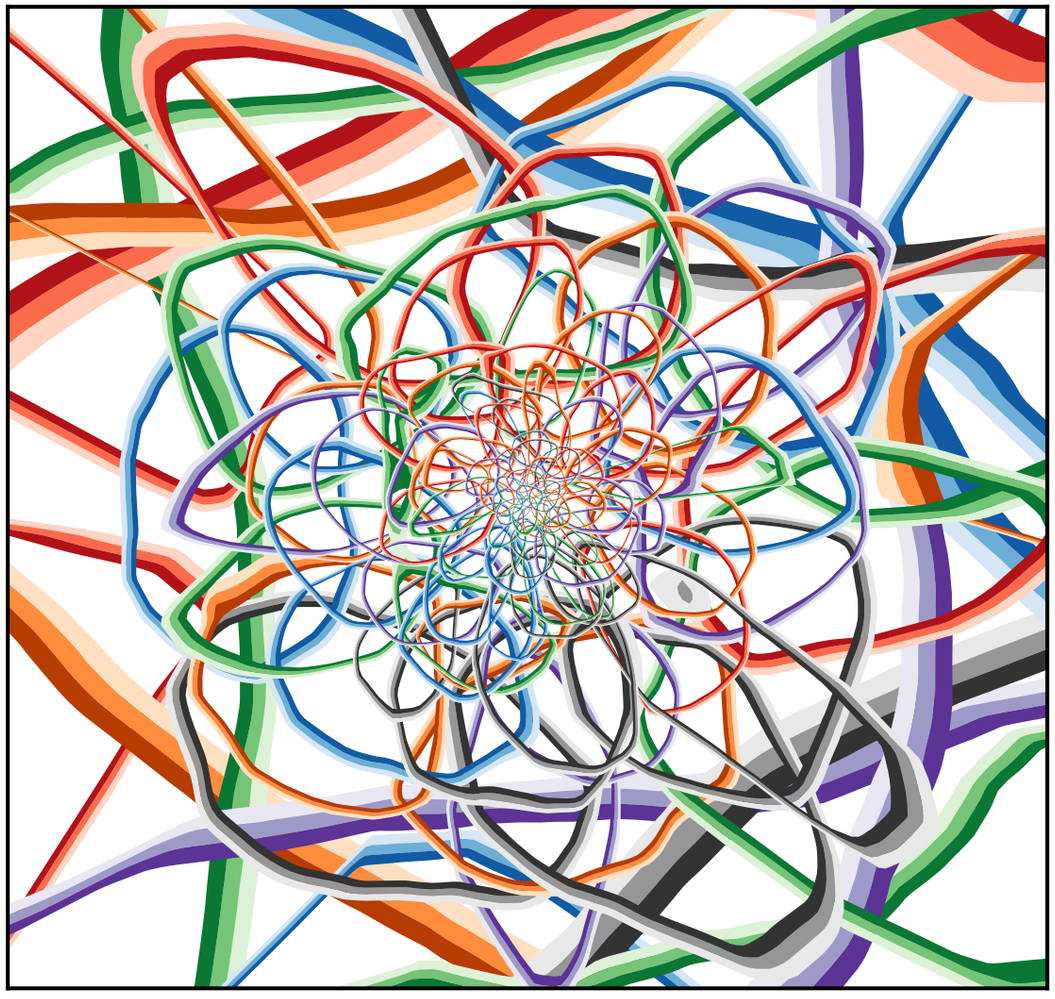


Latent Dimension 64

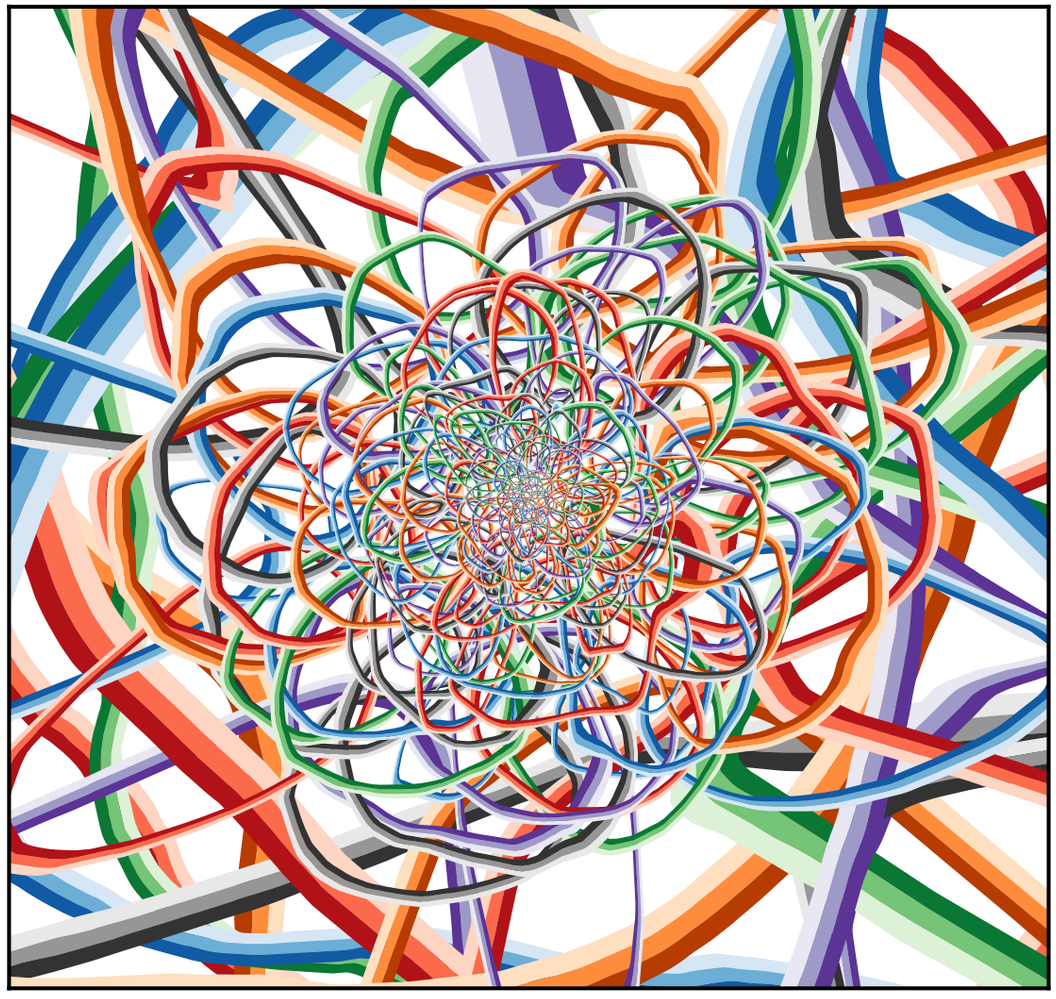


# Psychedelic Network Visualization

Latent Dimension 128

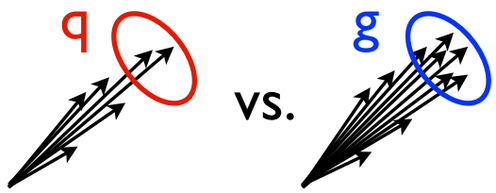


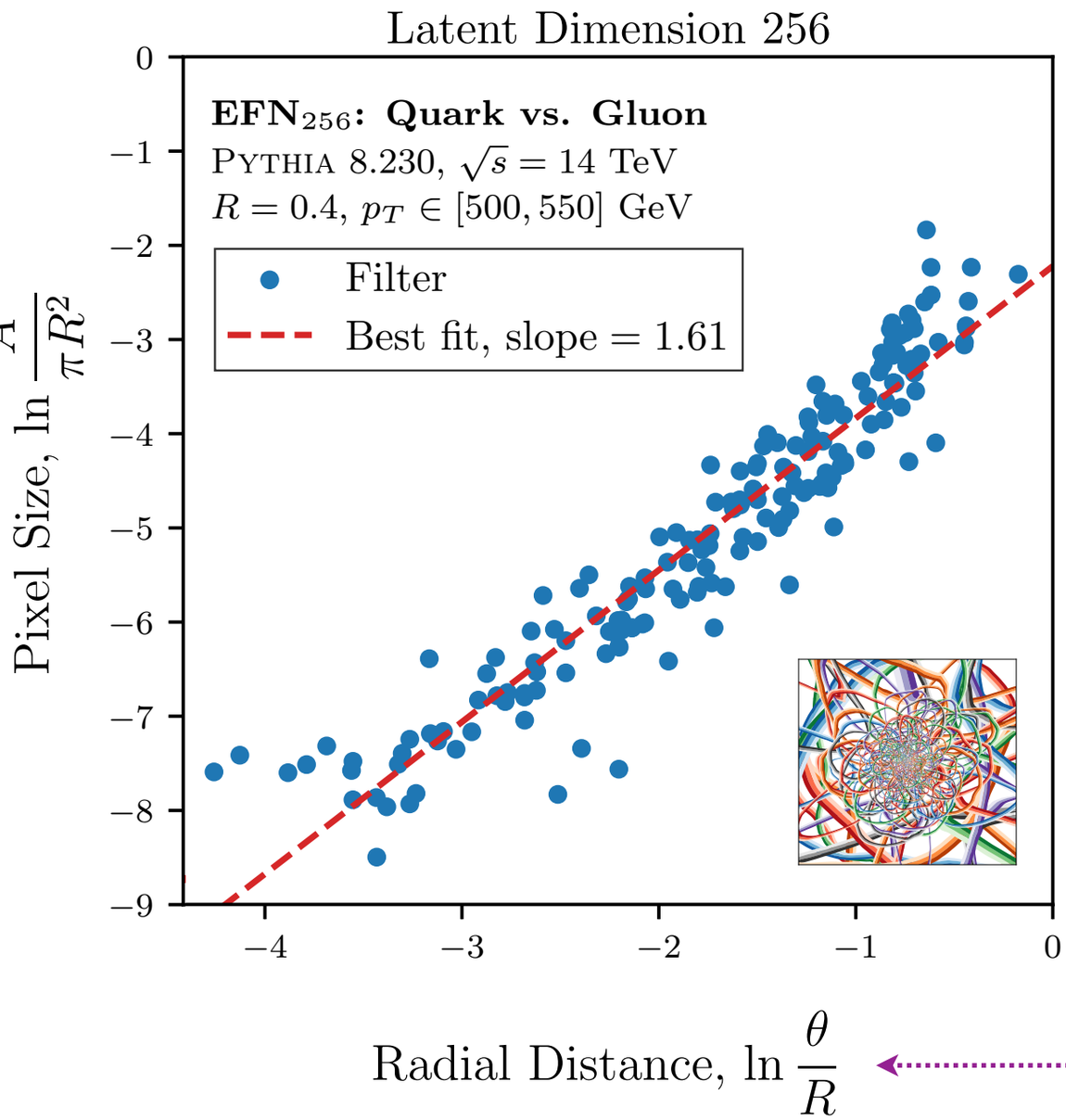
Latent Dimension 256

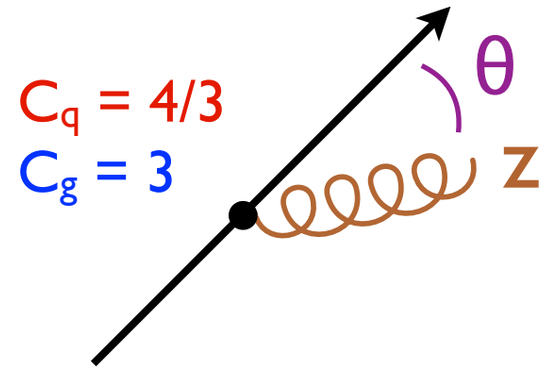


*Singularity structure of QCD!*

# Putting the AI in AItarelli-Parisi



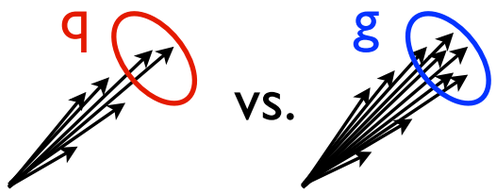



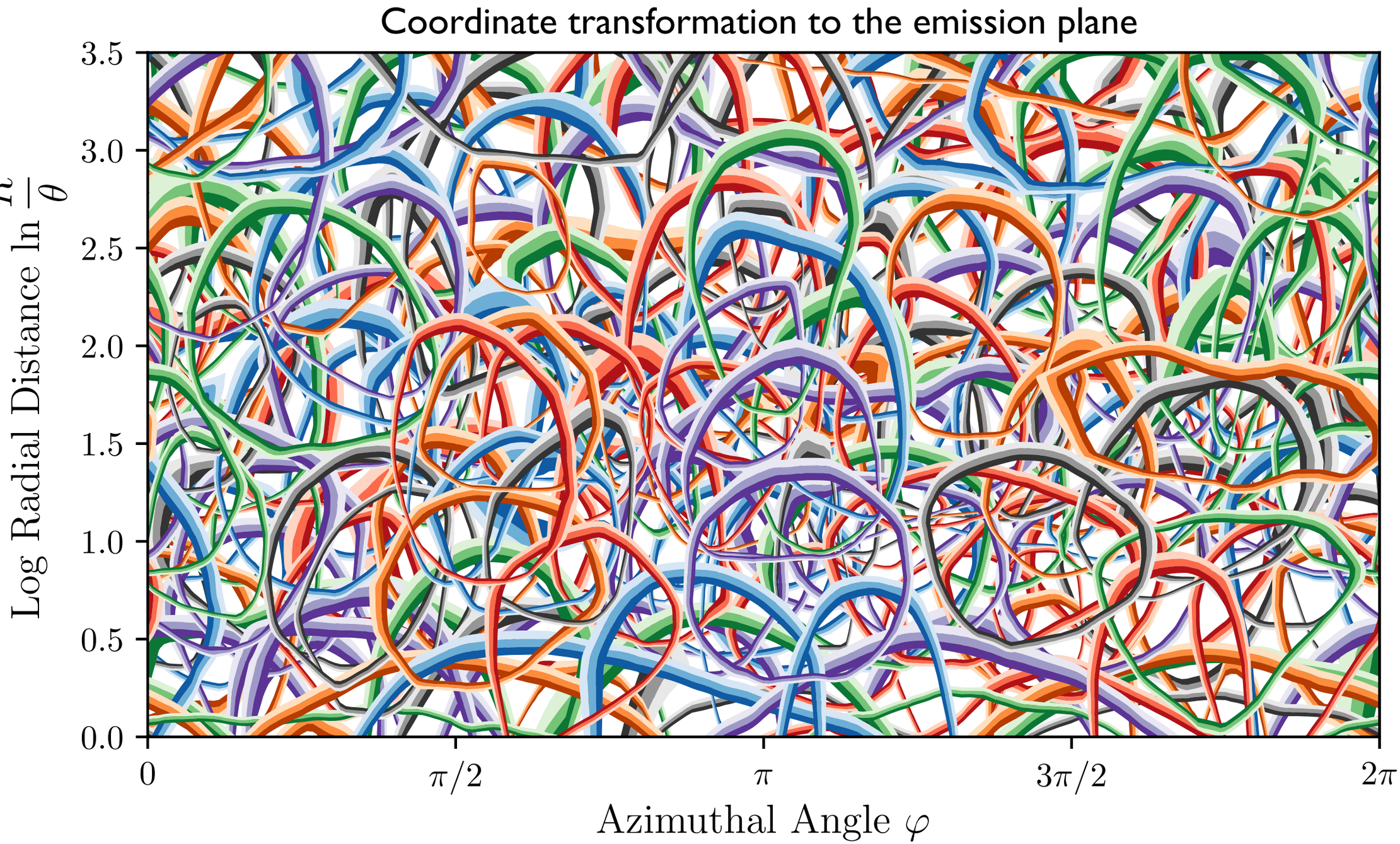

$$\mathrm{d}P_{i\to ig} \simeq \frac{2\alpha_s}{\pi} C_i \frac{\mathrm{d}\theta}{\theta} \frac{\mathrm{d}z}{z}$$

Collinear Soft

[Komiske, Metodiev, JDT, JHEP 2019]

# Ready for the Hirshhorn?



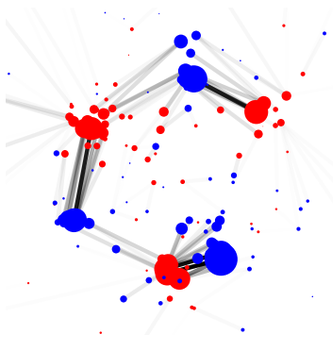




[Komiske, Metodiev, JDT, JHEP 2019; see also Dreyer, Salam, Soyez, JHEP 2018]

# Particle Physics 101



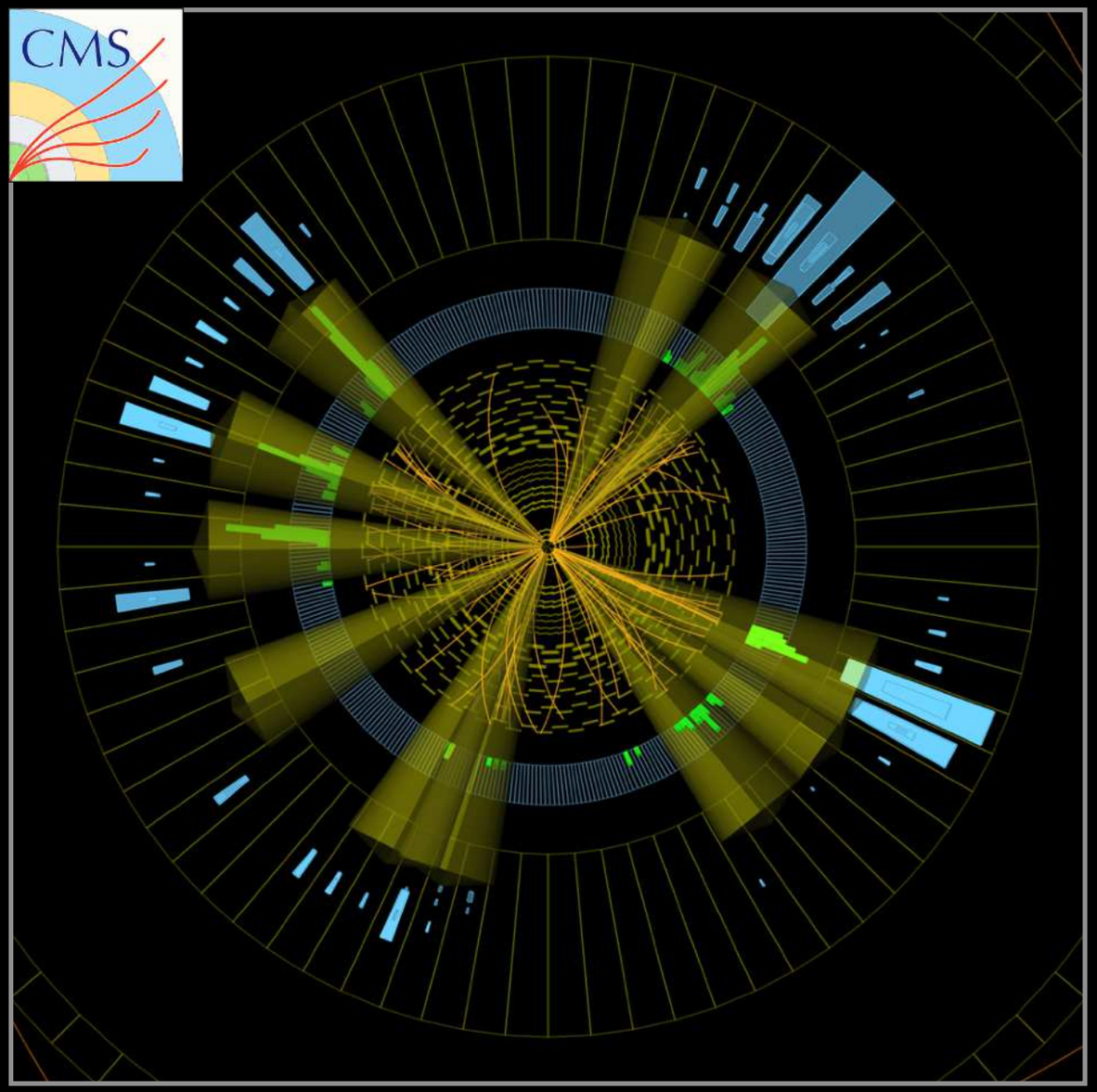
## What is a Collider Event?

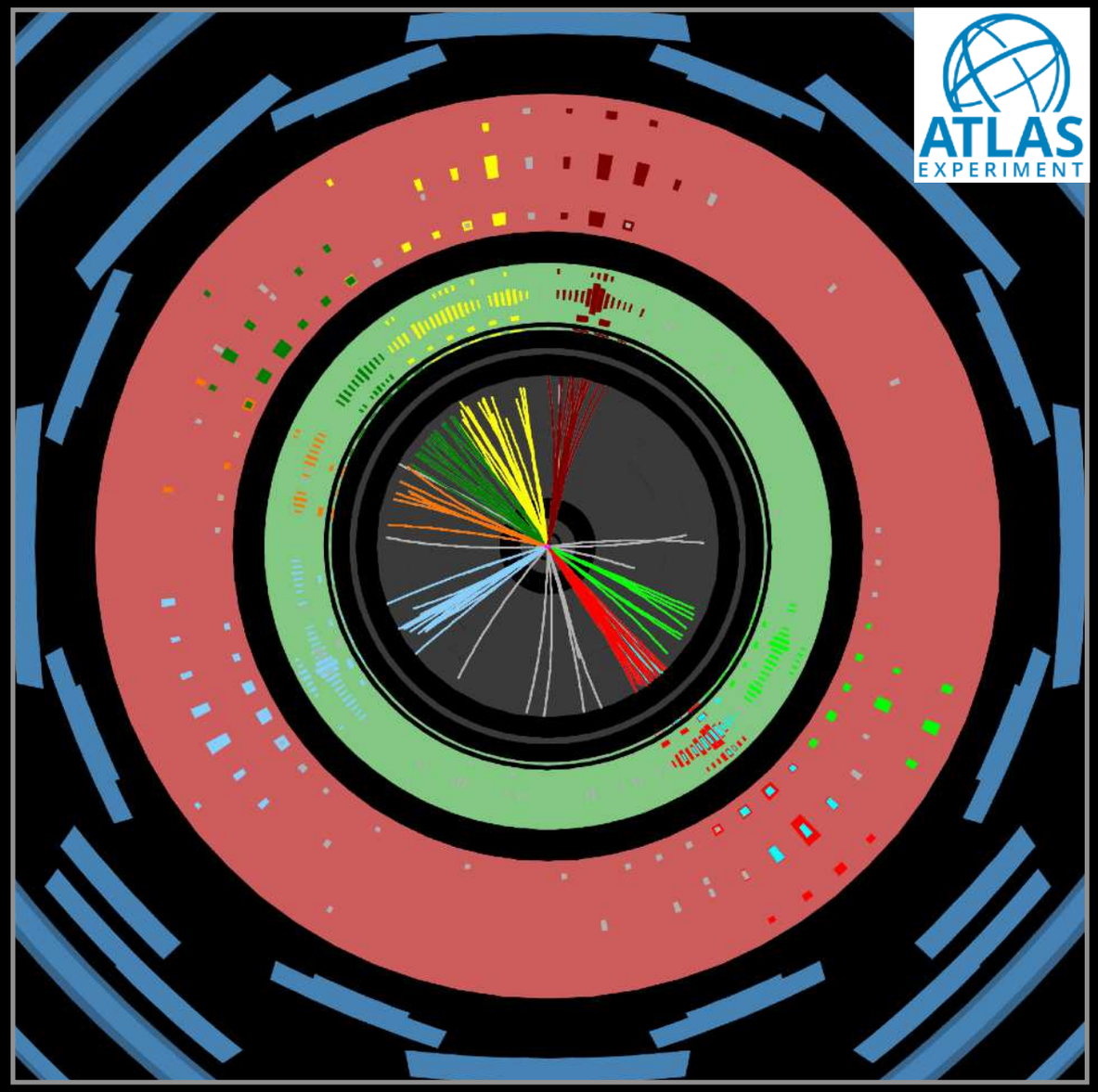


## When are Collider Events Similar?

# *Two Collider Events*

Two collections of points in (momentum) space

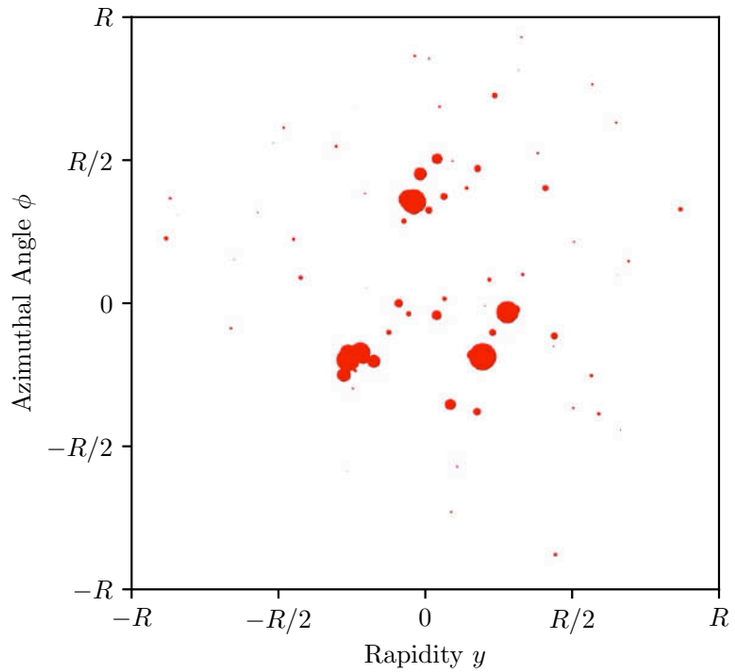



*How "close" are these? (8.5 km?)*

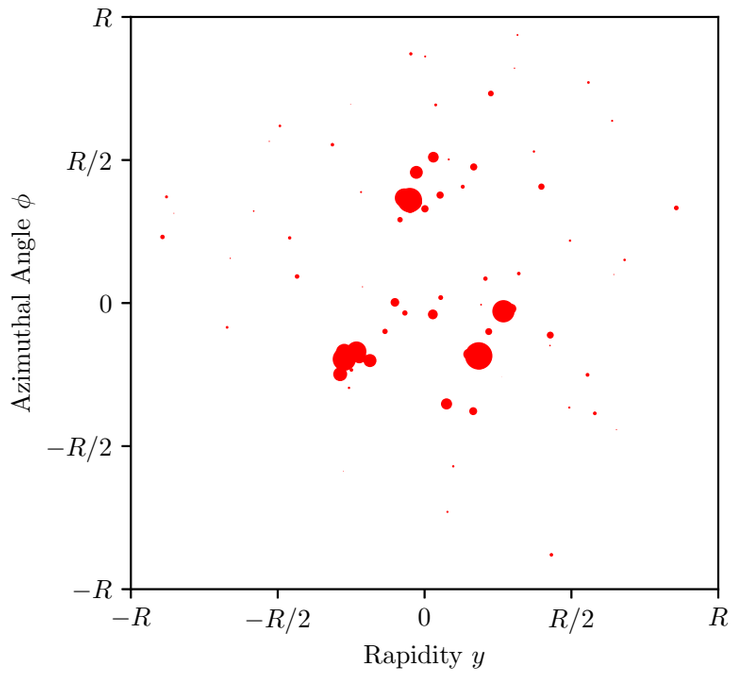
# Similarity of Two Energy Flows?

$$\mathcal{E}(\hat{n}) = \sum_i E_i \, \delta(\hat{n} - \hat{n}_i)$$

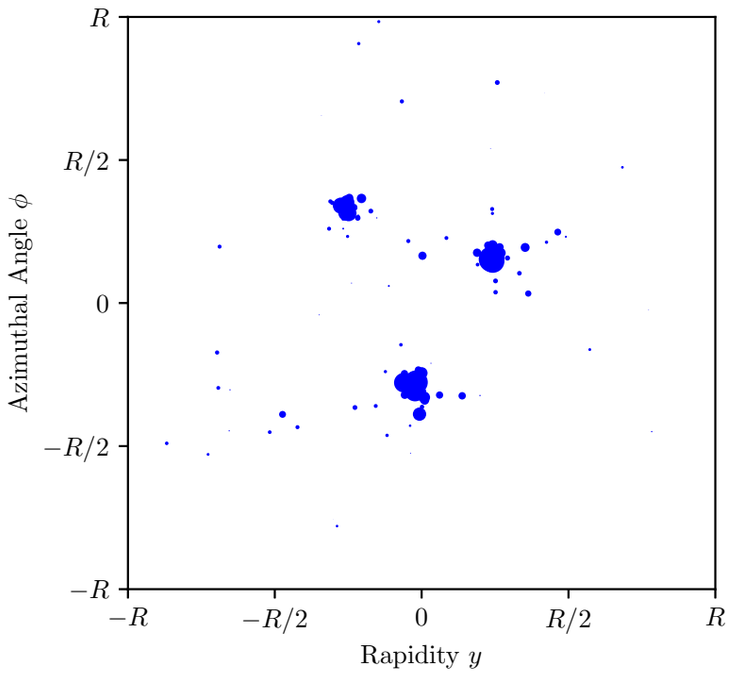



## Optimal Transport:

*Earth Mover's Distance*
*a.k.a. 1-Wasserstein metric*




125.4 GeV




[Komiske, Metodiev, JDT, PRL 2019; code at Komiske, Metodiev, JDT, energyflow.network]

# The Earth Mover's Distance

## Optimal Transport:

[Peleg, Werman, Rom, IEEE 1989;
Rubner, Tomasi, Guibas, ICCV 1998, ICJV 2000;
Pele, Werman, ECCV 2008; Pele Taskar, GSI 2013]

Minimum "work" (stuff x distance) to make one distribution look like another distribution

Déblai

Remblai

[h/t Niles-Weed, ML4Jets 2020; Monge, 1781; Vaserštein, 1969; Wikipedia]

# The Earth Mover's Distance

Optimal Transport:

[Peleg, Werman, Rom, IEEE 1989;
Rubner, Tomasi, Guibas, ICCV 1998, ICJV 2000;
Pele, Werman, ECCV 2008; Pele Taskar, GSI 2013]

Minimum "work" (stuff x distance) to make one distribution look like another distribution

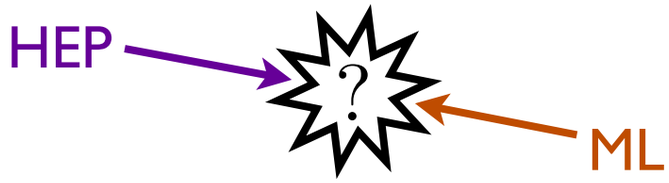
Additive Weight: ●

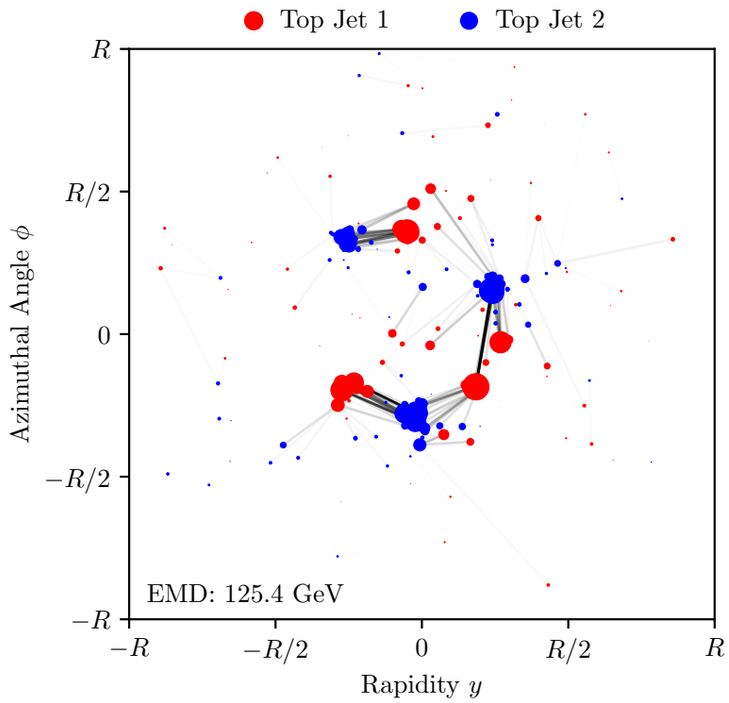
Ground Distance: ⟷

$\Rightarrow$ Distance Between Distributions

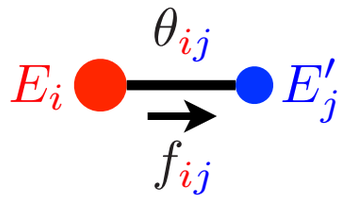

[h/t Niles-Weed, ML4Jets 2020; Monge, 1781; Vaserštein, 1969; Wikipedia]

# The Energy Mover's Distance




Optimal transport of energy flows…

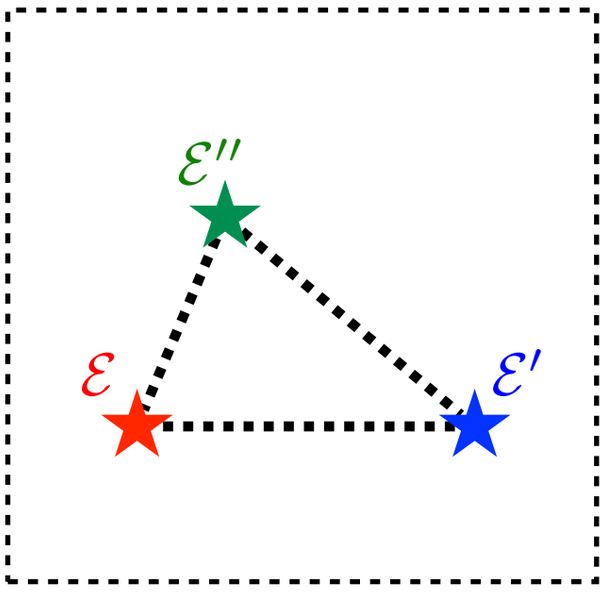



$$\mathrm{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f\}} \sum_i \sum_j f_{ij} \frac{\theta_{ij}}{R} + \left| \sum_i E_i - \sum_j E'_j \right|$$

in GeV

Cost to move energy

Cost to create energy




…defines a metric on the space of events

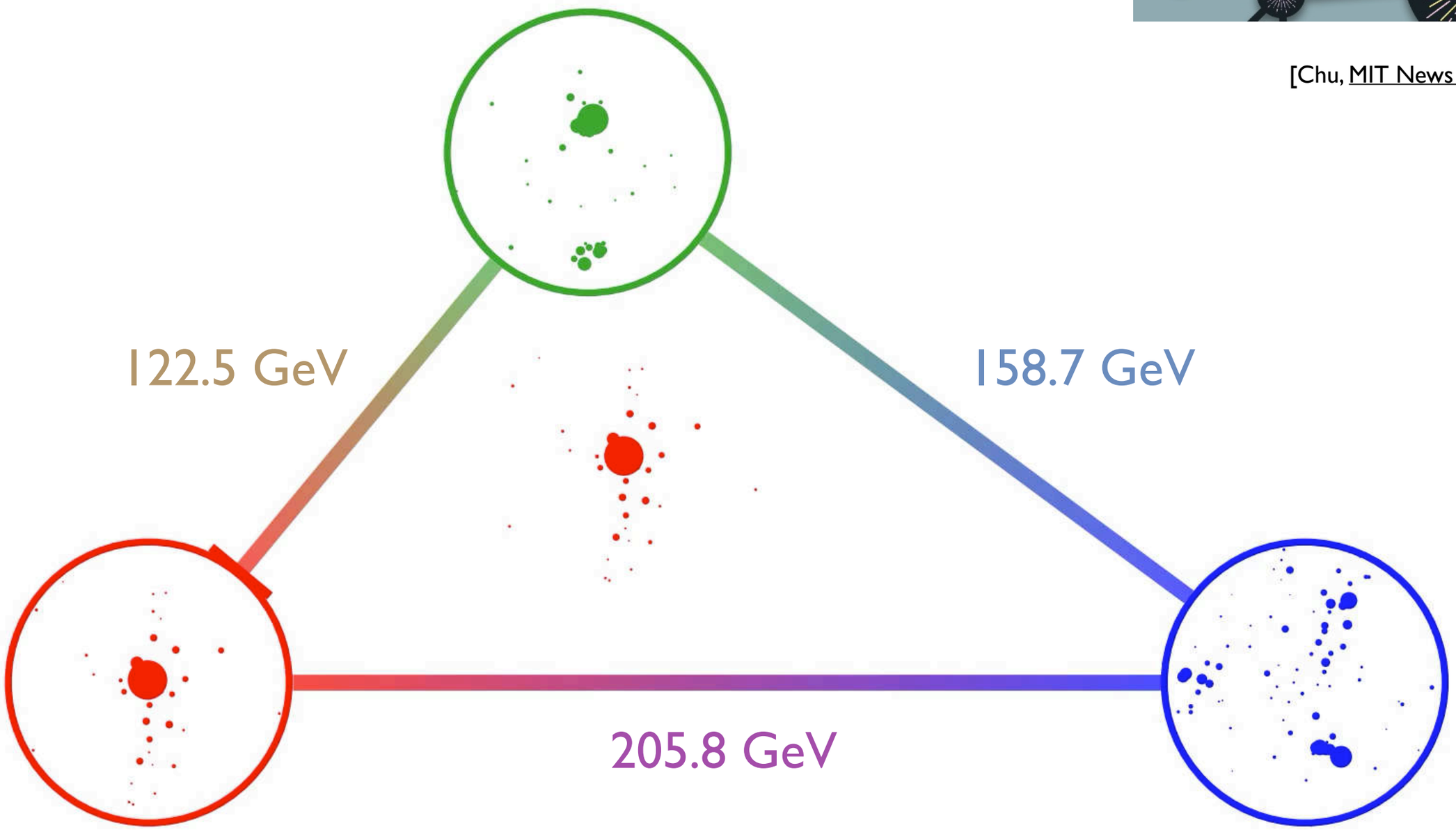
$$0 \leq \mathrm{EMD}(\mathcal{E}, \mathcal{E}') \leq \mathrm{EMD}(\mathcal{E}, \mathcal{E}'') + \mathrm{EMD}(\mathcal{E}', \mathcal{E}'')$$

(assuming $R \geq \theta_{max}/2$, i.e. R ≥ jet radius for conical jets)

[Komiske, Metodiev, JDT, PRL 2019;
see also Pele, Werman, ECCV 2008; Pele, Taskar, GSI 2013;
see flavored variant in Crispim Romão, Castro, Milhano, Pedro, Vale, arXiv 2020]

# Triangulating the Space of Jets

[Chu, MIT News July 2019]




[Komiske, Metodiev, JDT, PRL 2019; code at Komiske, Metodiev, JDT, energyflow.network]

# Dimensionality of Space of Jets

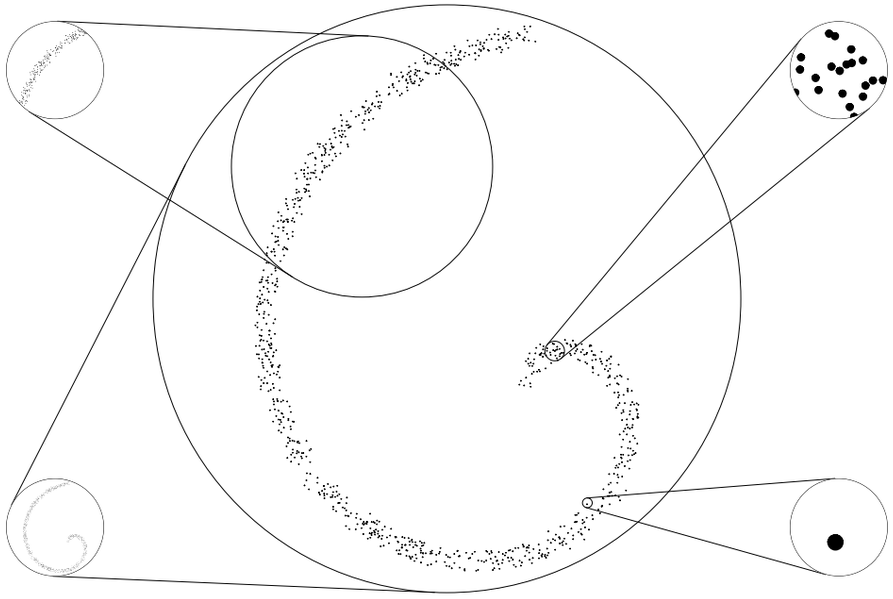
$$N_{\text{neighbors}}(r) \sim r^{\dim}$$

$$\Rightarrow \quad \dim(r) \sim r \frac{\partial}{\partial r} \ln N_{\text{neighbors}}(r)$$

[Grassberger, Procaccia, PRL 1983; Kégl, NIPS 2002]

dim≃1

dim≃2



dim≃2

(eventually 0)

dim≃0

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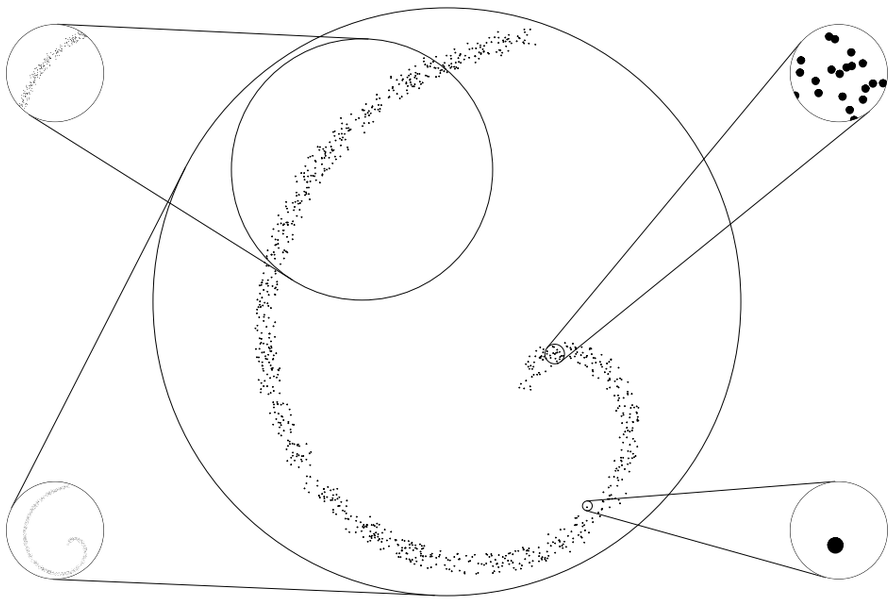
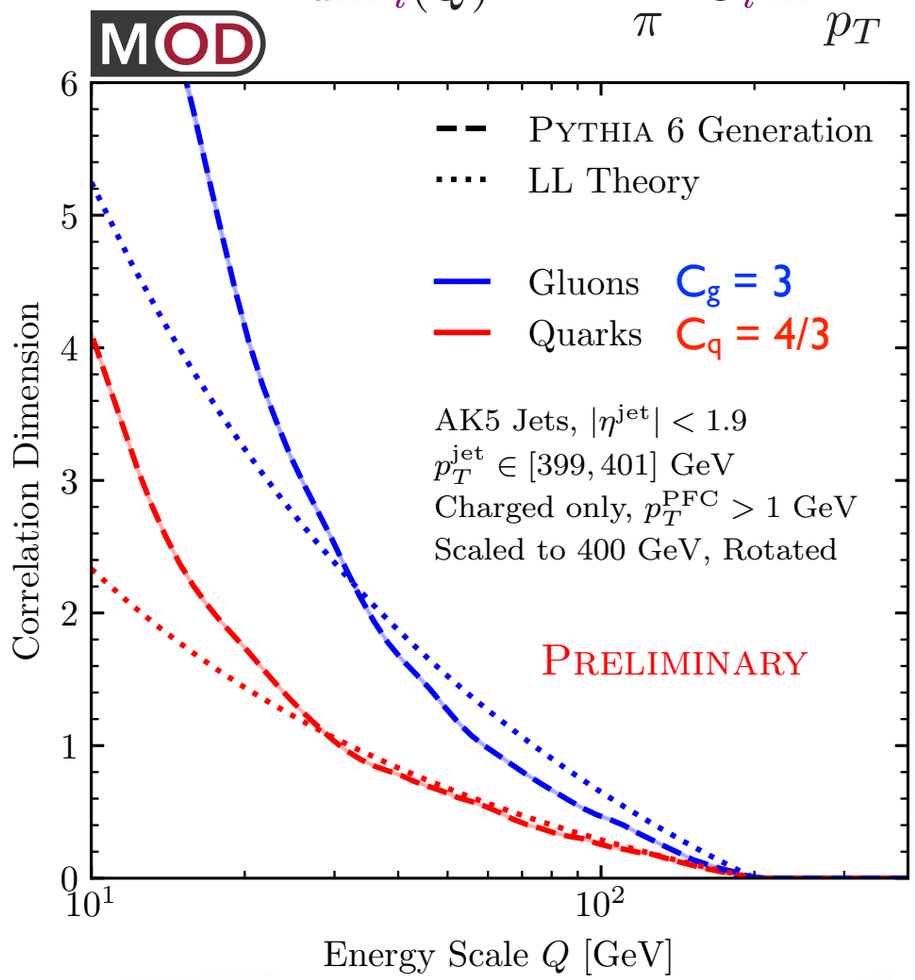


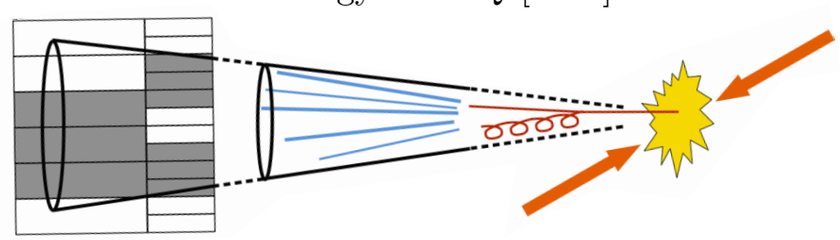
dim≃2

(eventually 0)

dim≃0

$$\dim_i(Q) \simeq -\frac{8\alpha_s}{\pi} C_i \ln \frac{Q}{p_T}$$



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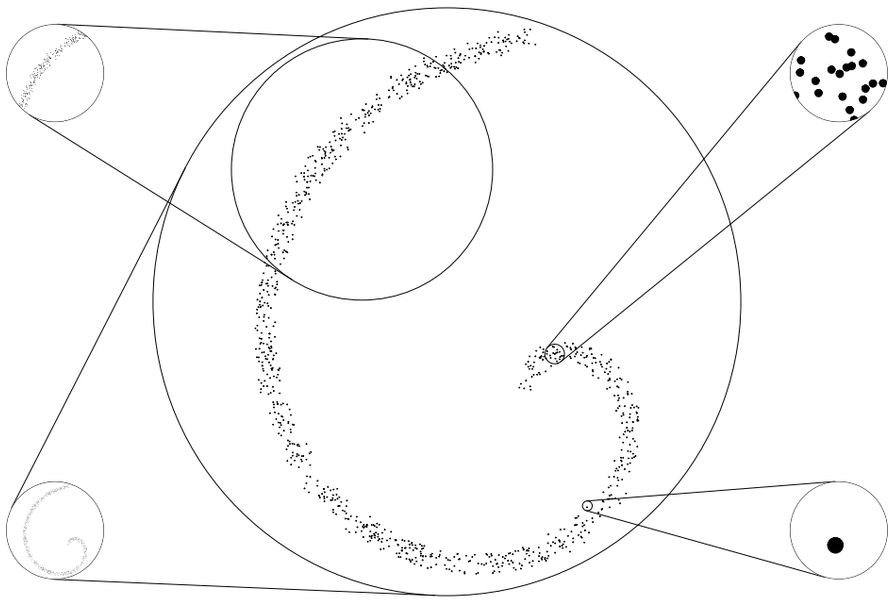
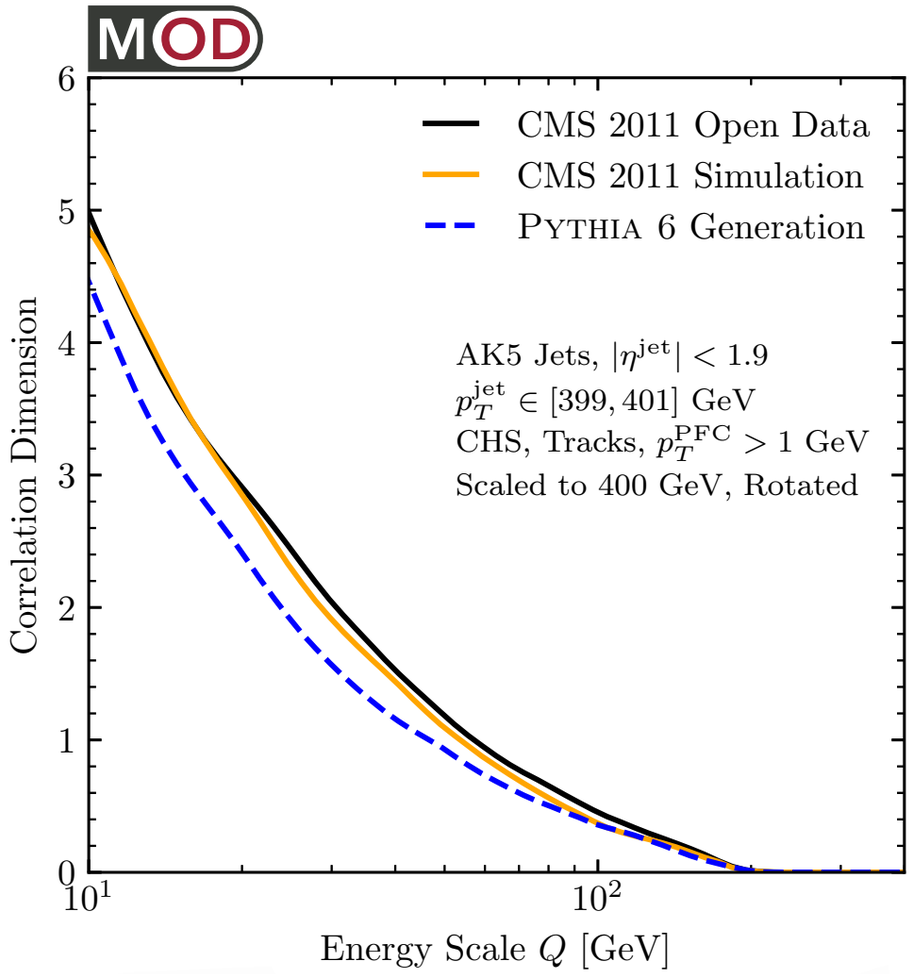
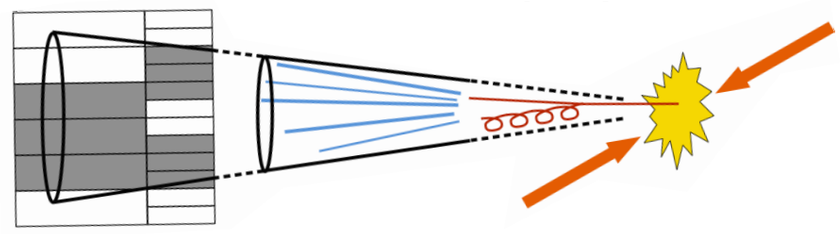


dim≃2

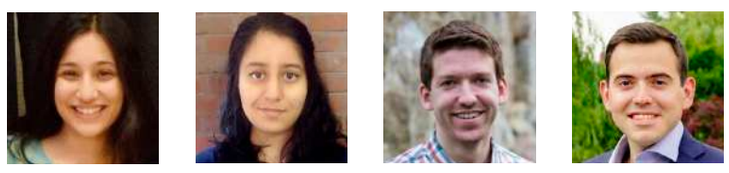
(eventually 0)

dim≃0

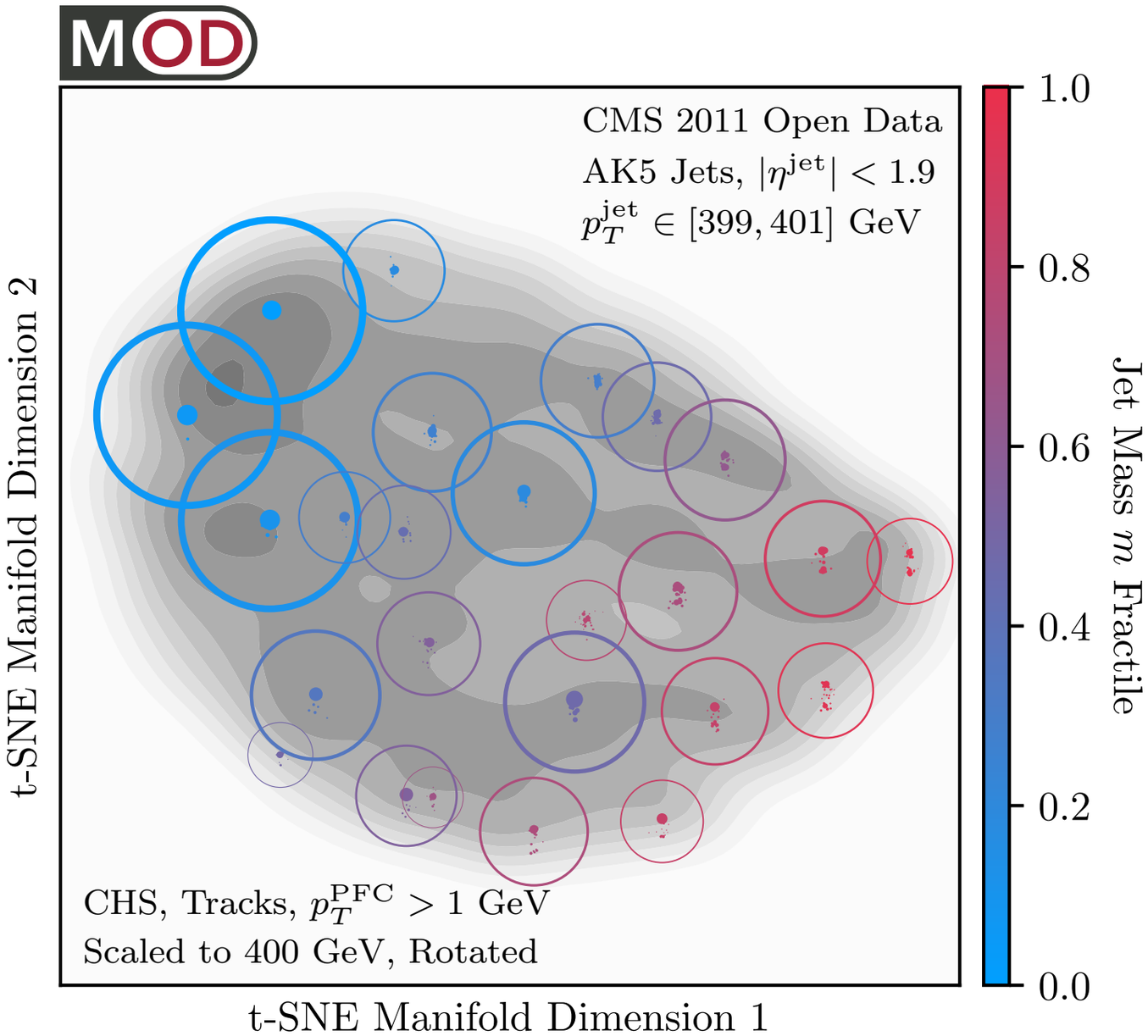


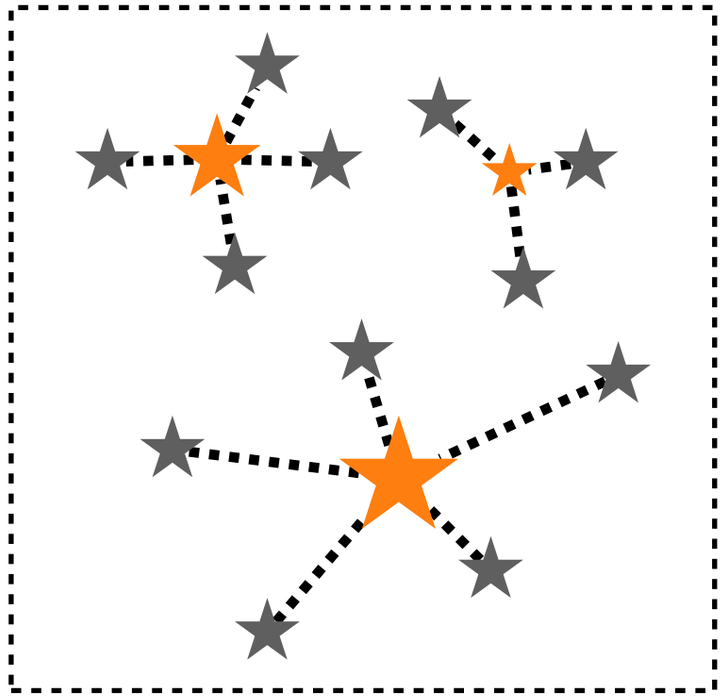



[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020; using CMS Open Data]



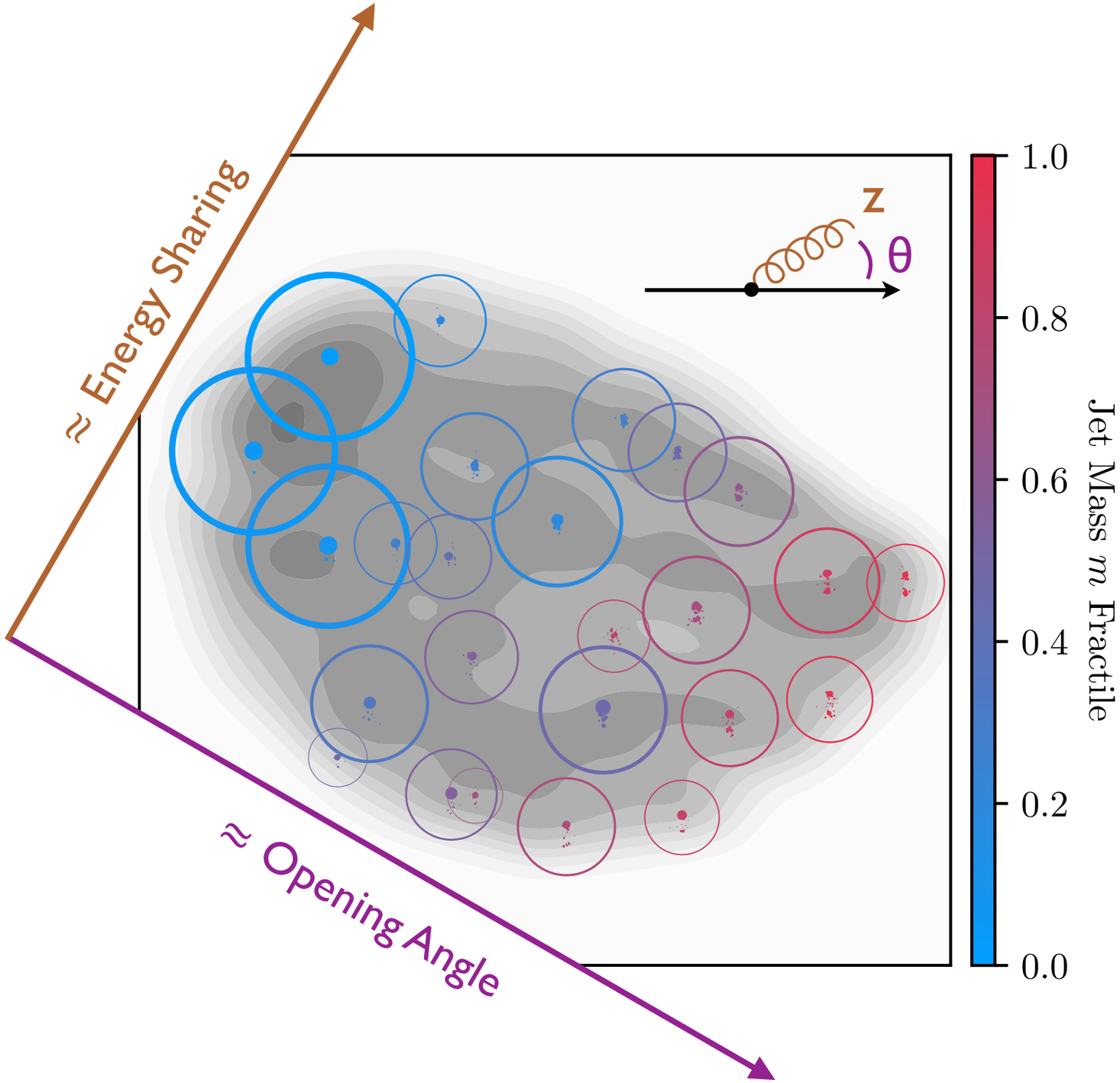
# Most Representative Jets



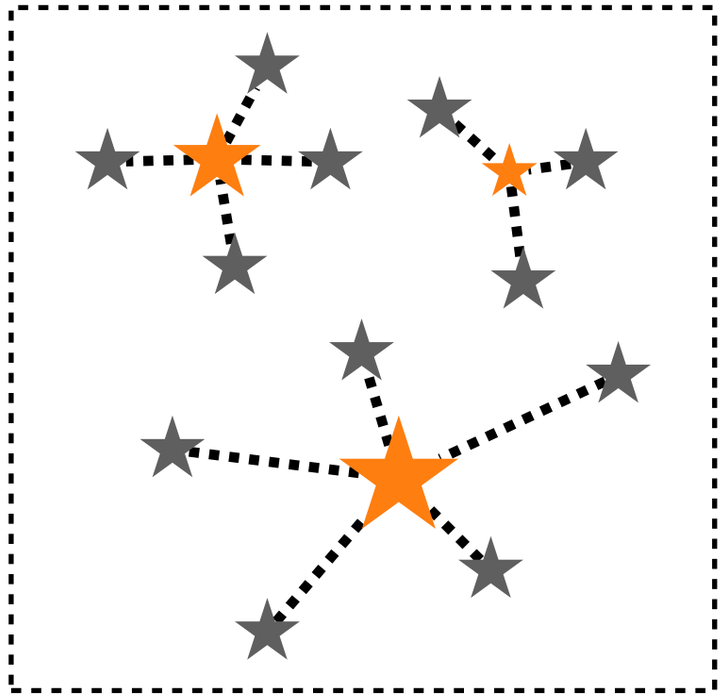

[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020; using van der Maaten, Hinton, JMLR 2008]

# Most Representative Jets



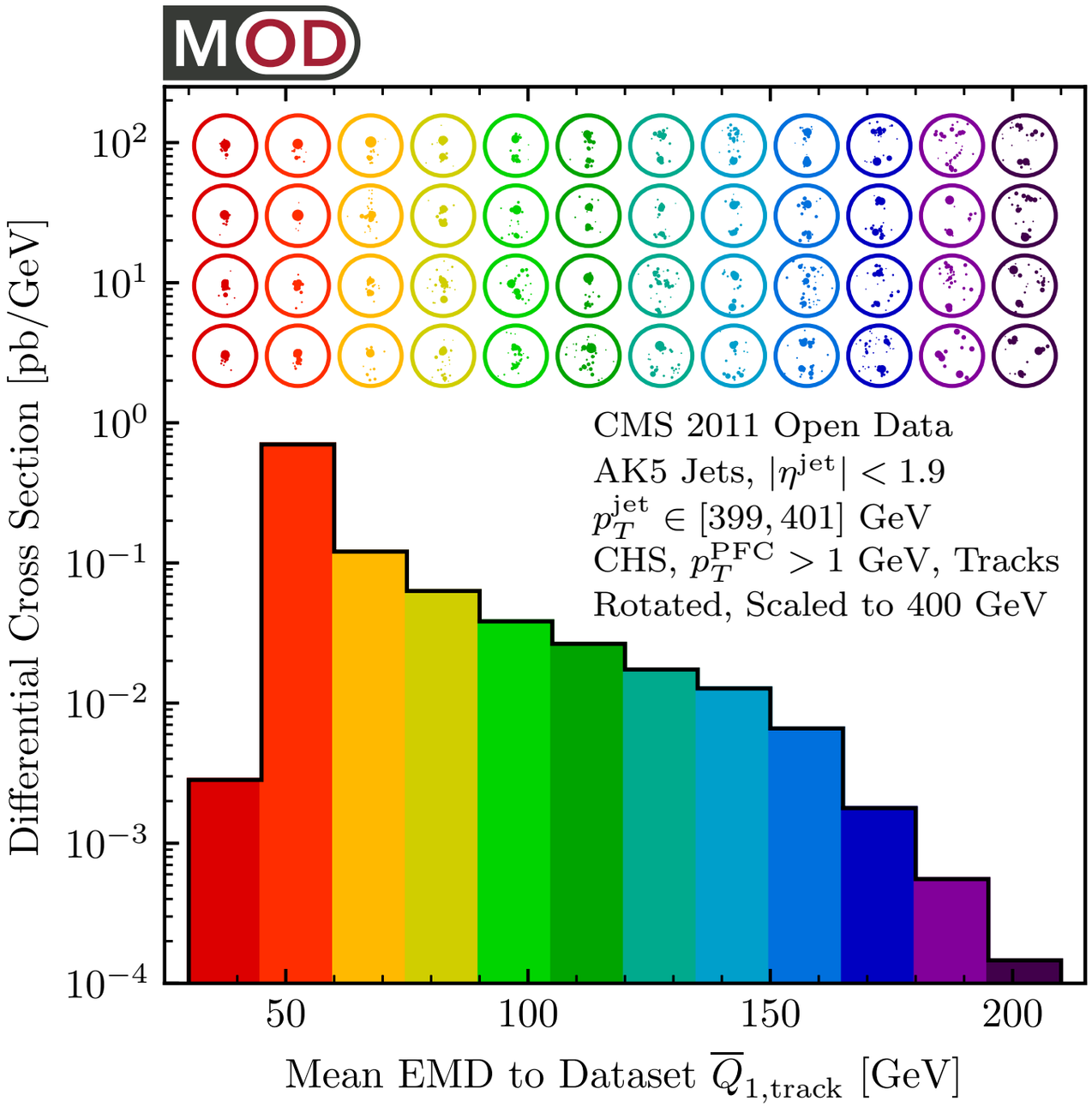

## k-medoids

*Arranged via t-SNE*



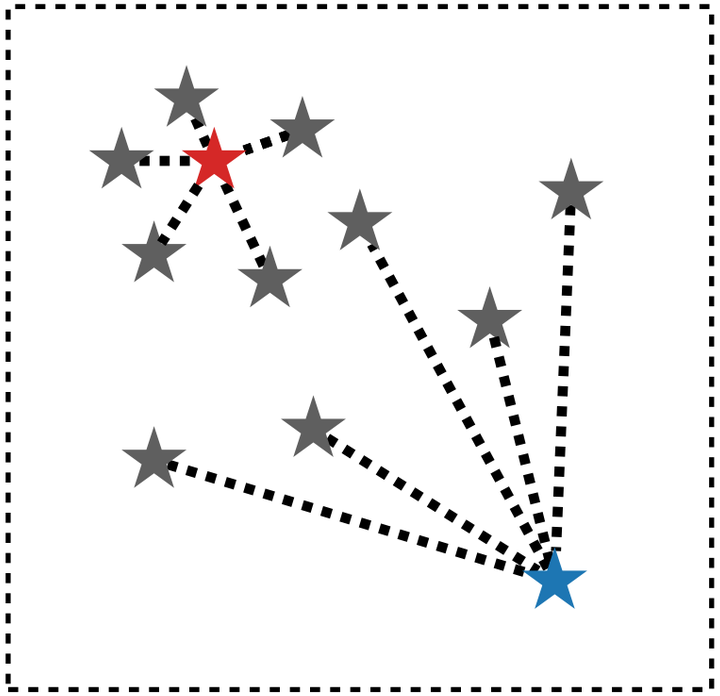
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020; using van der Maaten, Hinton, JMLR 2008]

# Least Representative Jets




## New Physics?

*Or tails of QCD?*

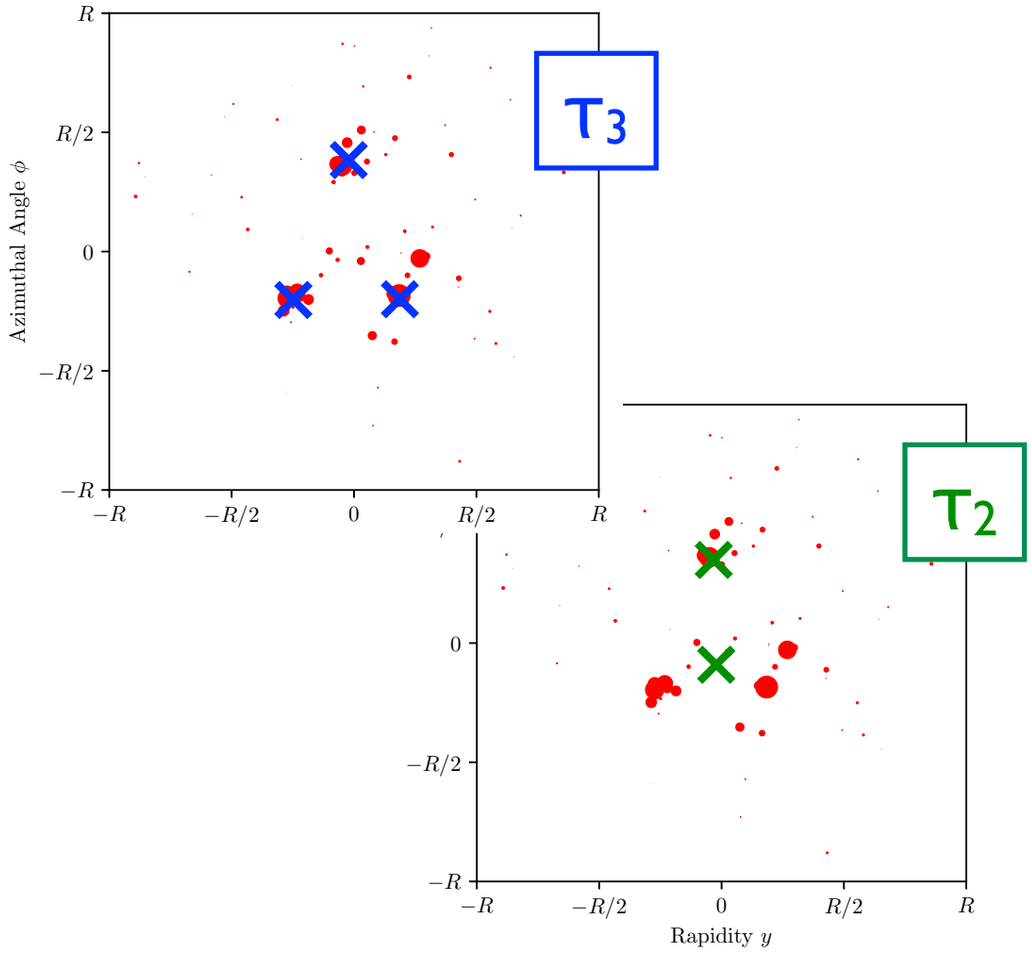


[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020]

# N-subjettiness

*Ubiquitous jet substructure observable used for almost a decade…*

$$\tau_N(\mathcal{J}) = \min_{N \text{ axes}} \sum_i E_i \min\{\theta_{1,i}, \theta_{2,i}, \ldots, \theta_{N,i}\}$$

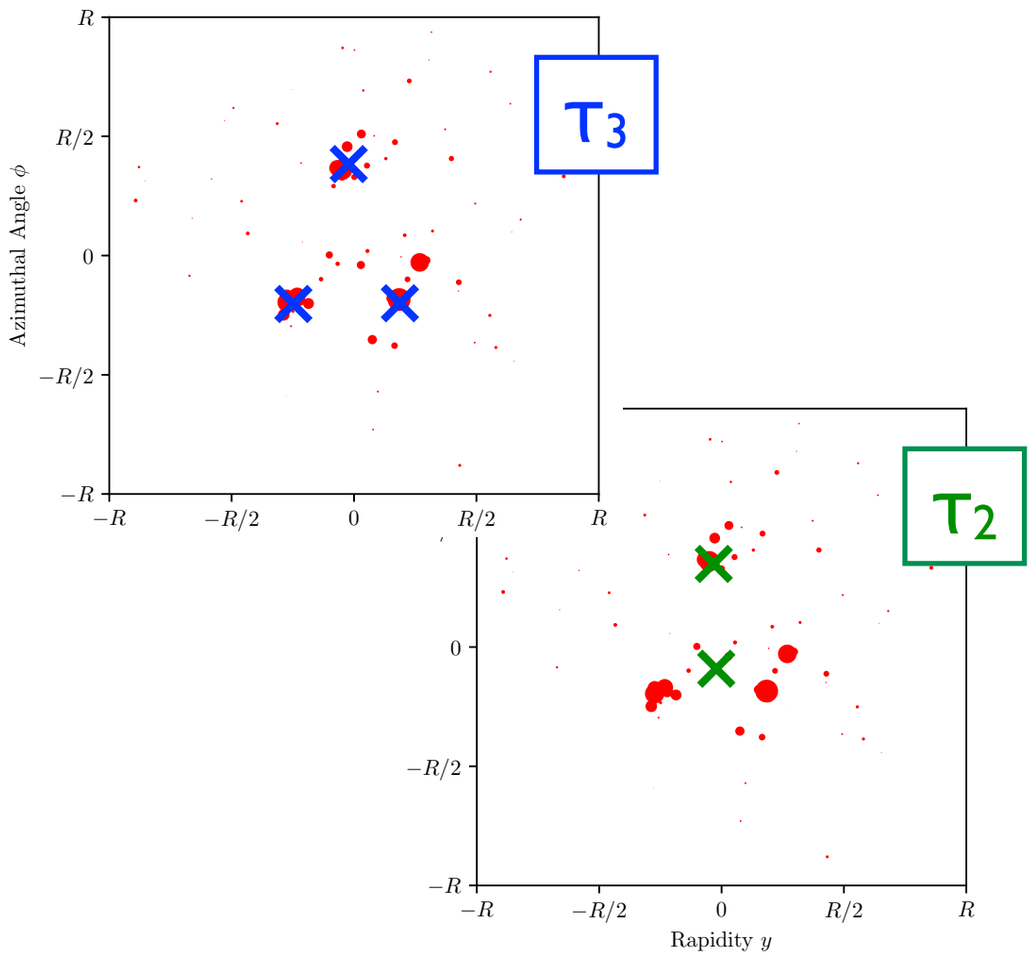


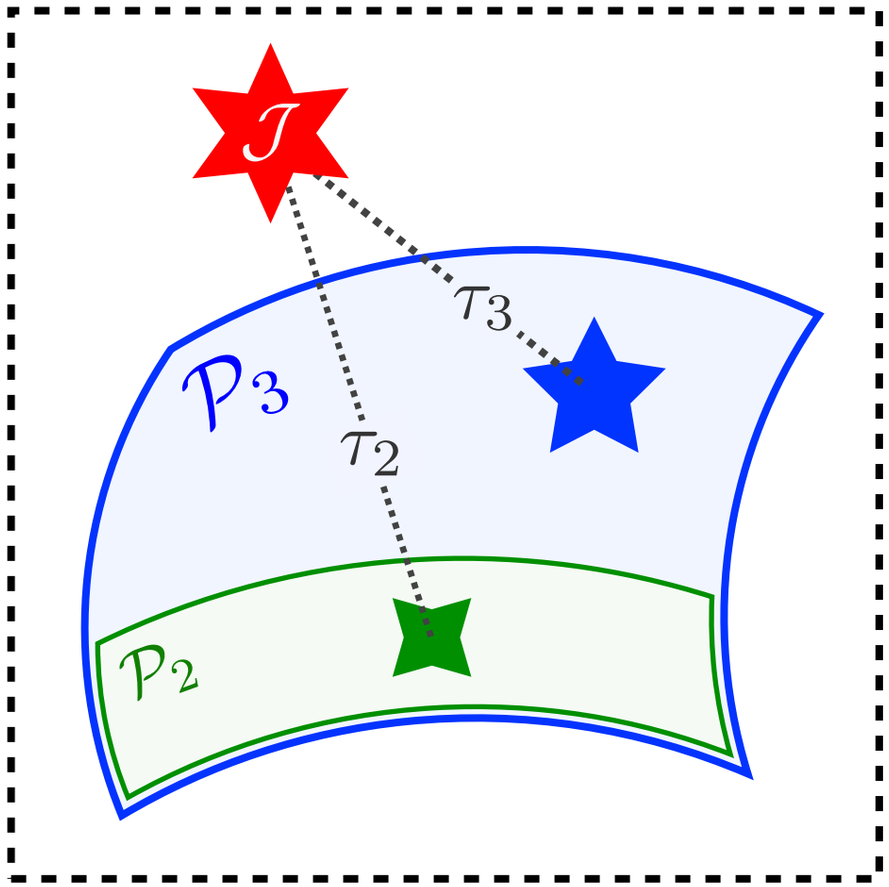

[JDT, Van Tilburg, JHEP 2011, JHEP 2012;
based on Brandt, Dahmen, ZPC 1979; Stewart, Tackmann, Waalewijn, PRL 2010]

# N-subjettiness = Point to Manifold EMD

*…is secretly an optimal transport problem*

$$\tau_N(\mathcal{J}) = \min_{\mathcal{J}' \in \mathcal{P}_N} \mathrm{EMD}(\mathcal{J}, \mathcal{J}')$$

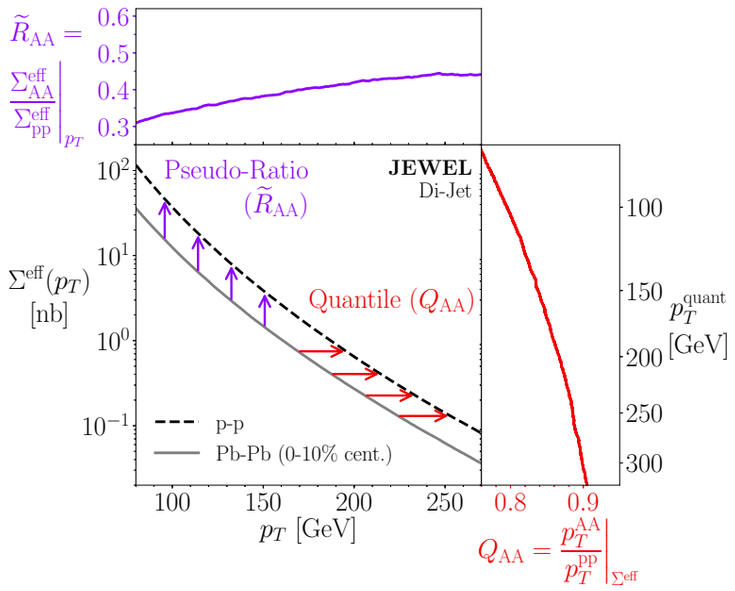



[JDT, Van Tilburg, JHEP 2011, JHEP 2012;
rephrased via Komiske, Metodiev, JDT, JHEP 2020; see opposite limit in Cesarotti, JDT, JHEP 2020]

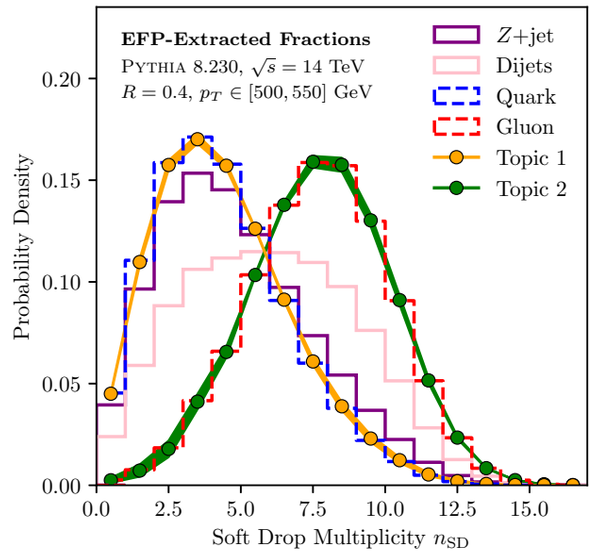
# More Collisions


## Jet Quenching via Optimal Transport




[Brewer, Milhano, JDT, PRL 2019]

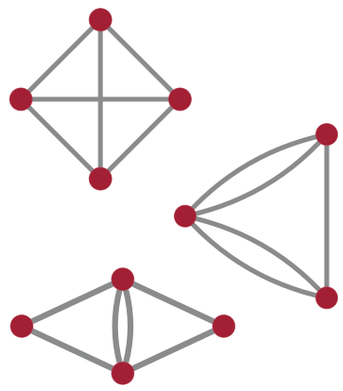
## Quark/Gluon Definitions via Blind Source Separation




[Komiske, Metodiev, JDT, JHEP 2018; Brewer, JDT, Turner; arXiv 2020]

## Kinematic Decomposition via Graph Theory

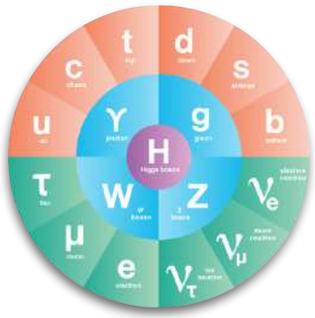
| Edges $d$ | Leafless Multigraphs Connected A307317 | All A307316 |
|---|---|---|
| 1 | 0 | 0 |
| 2 | 1 | 1 |
| 3 | 2 | 2 |
| 4 | 4 | 5 |
| 5 | 9 | 11 |
| 6 | 26 | 34 |
| 7 | 68 | 87 |
| 8 | 217 | 279 |
| 9 | **718** | **897** |
| 10 | **2 553** | **3 129** |
| 11 | **9 574** | **11 458** |
| 12 | **38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



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

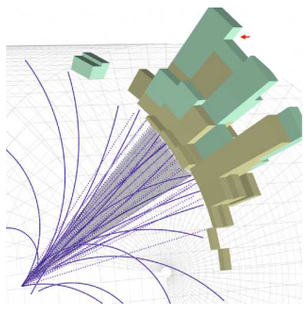
*New insights into particle physics**
*facilitated by advances in machine learning**

# Summary



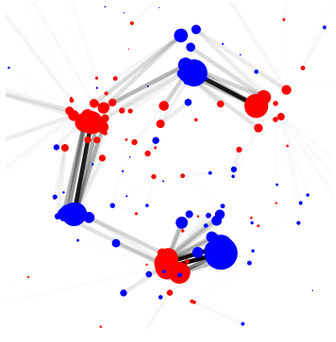

## Particle Physics 101

*High-energy collisions can yield insights into fundamental physics*
*Machine learning offers powerful tools to analyze collision debris*



## What is a Collider Event?

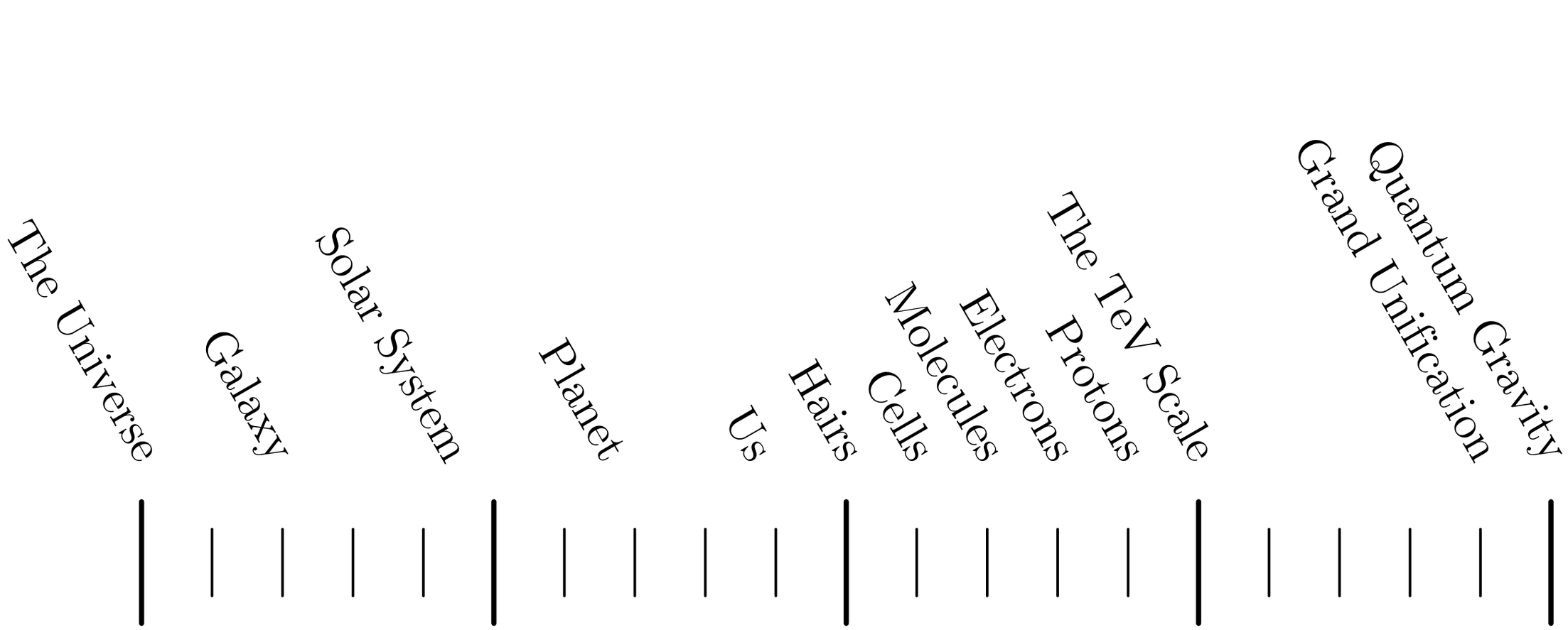
*Unordered set of particles describing energy flow of jets*
*Inspires network architectures designed for symmetry and safety*



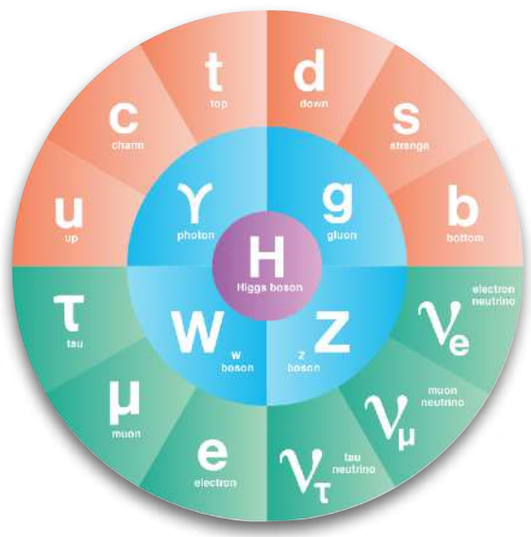
## When are Collider Events Similar?

*When their energy flows are similar*
*Inspires unsupervised learning strategies based on event geometry*

# *Backup Slides*




## The Standard Model



# Puzzles in Particle Physics

SnowMass2021

Matter/Anti-Matter?

Three Generations?

Strong CP?

Neutrino Masses?

*Compositeness?*
*Extra Dimensions?*
*Supersymmetry?*
*The Unexpected?*

$10^{26}$ m $10^{11}$ m $10^{-4}$ m $10^{-19}$ m $10^{-34}$ m

The Standard Model → ?

Grand Unification?

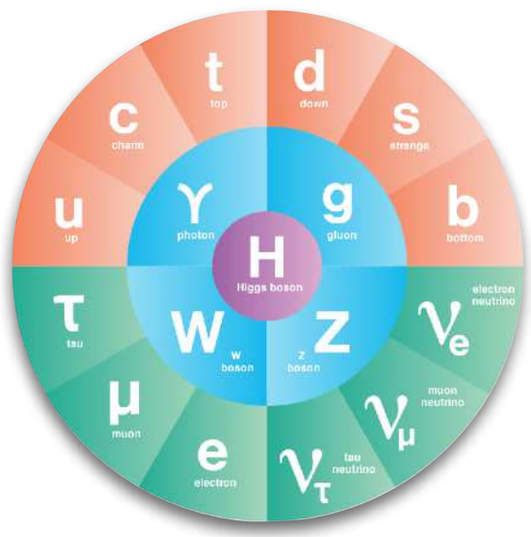
Dark Matter?

Origin of Mass?
Higgs Boson!

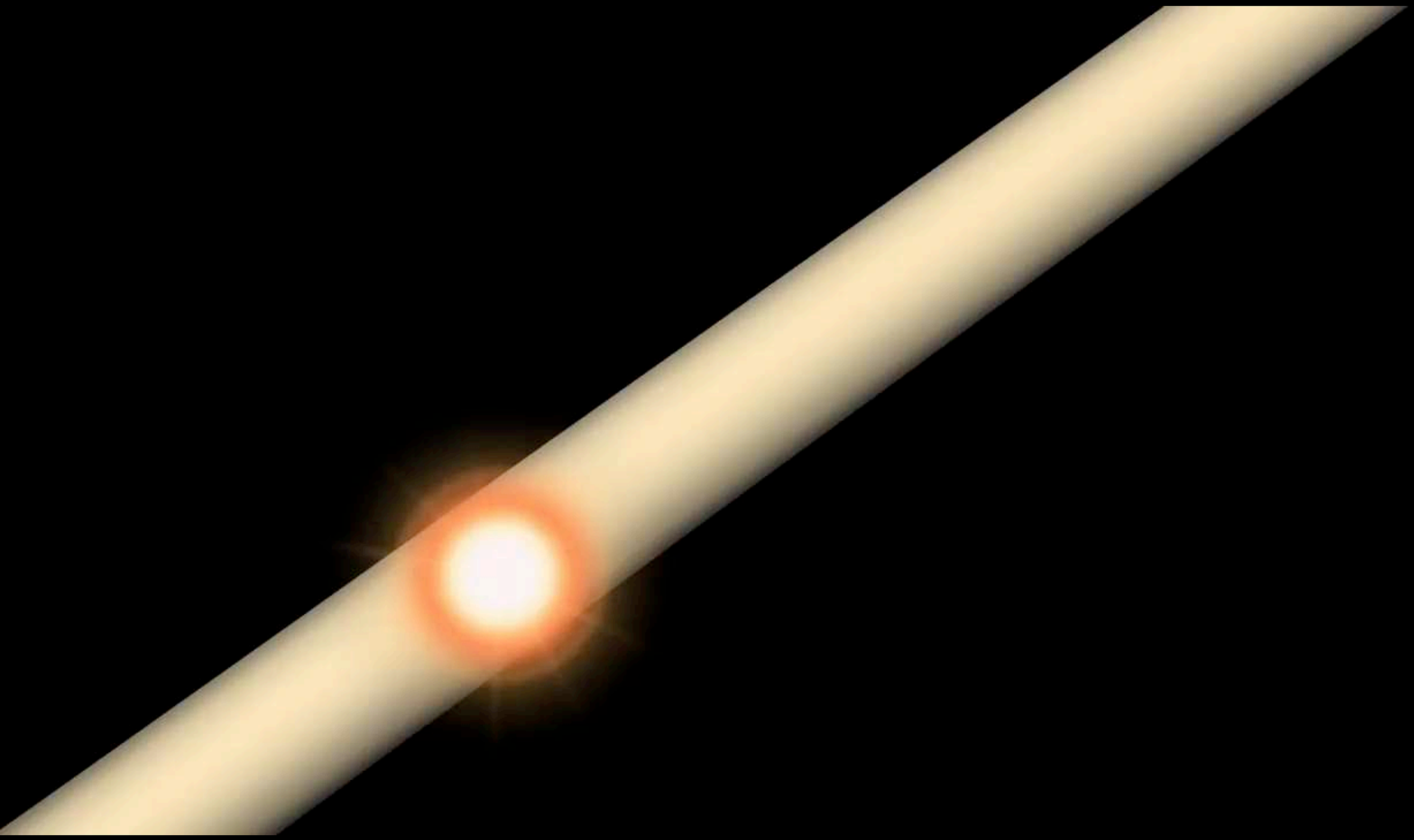
Quantum Gravity?

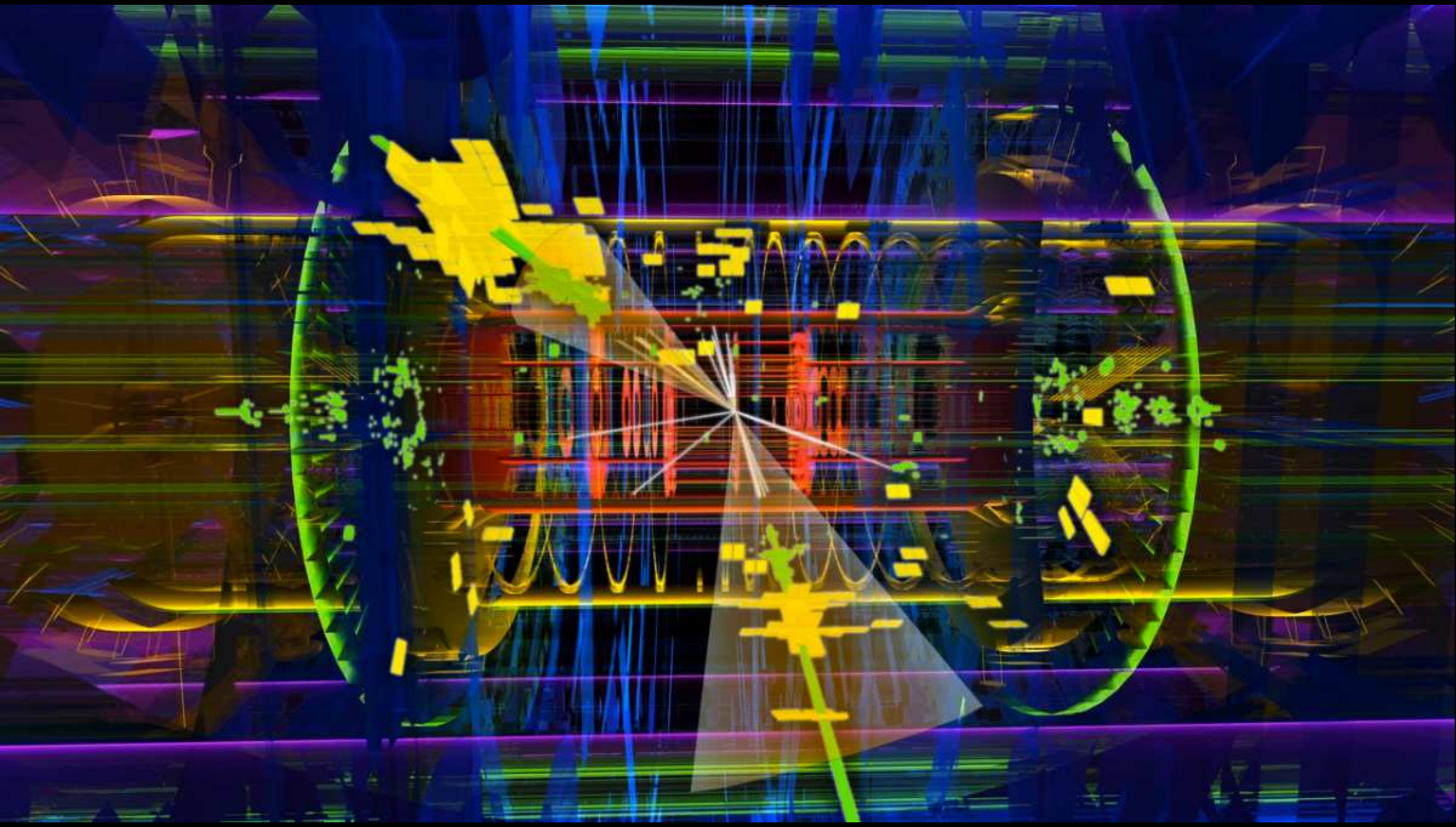
Dark Energy?

Inflation?



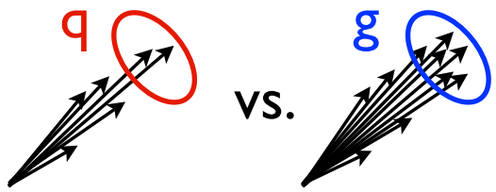

Hierarchy Problem?





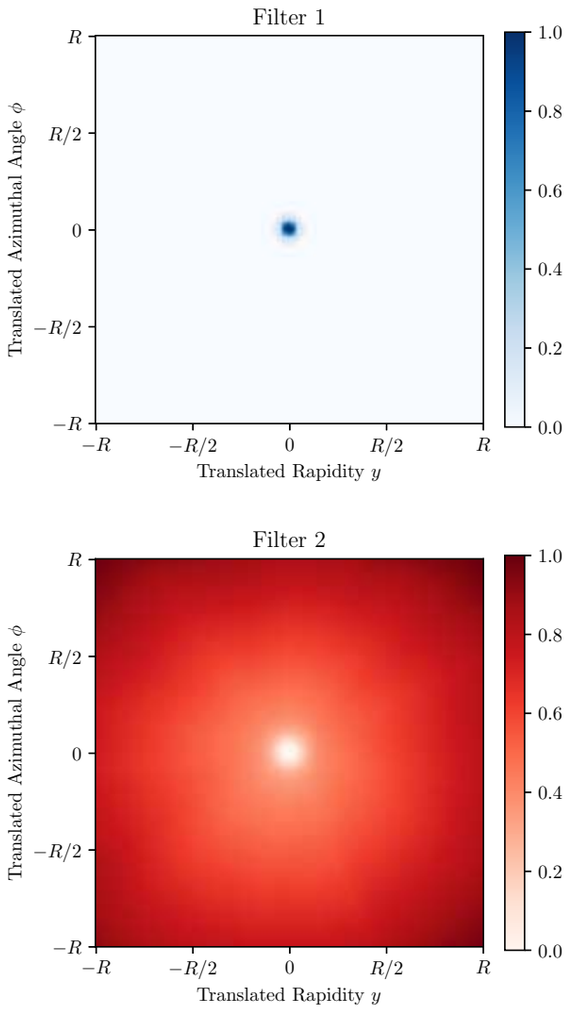
*"Ok, but did you really learn something you didn't already know?"*

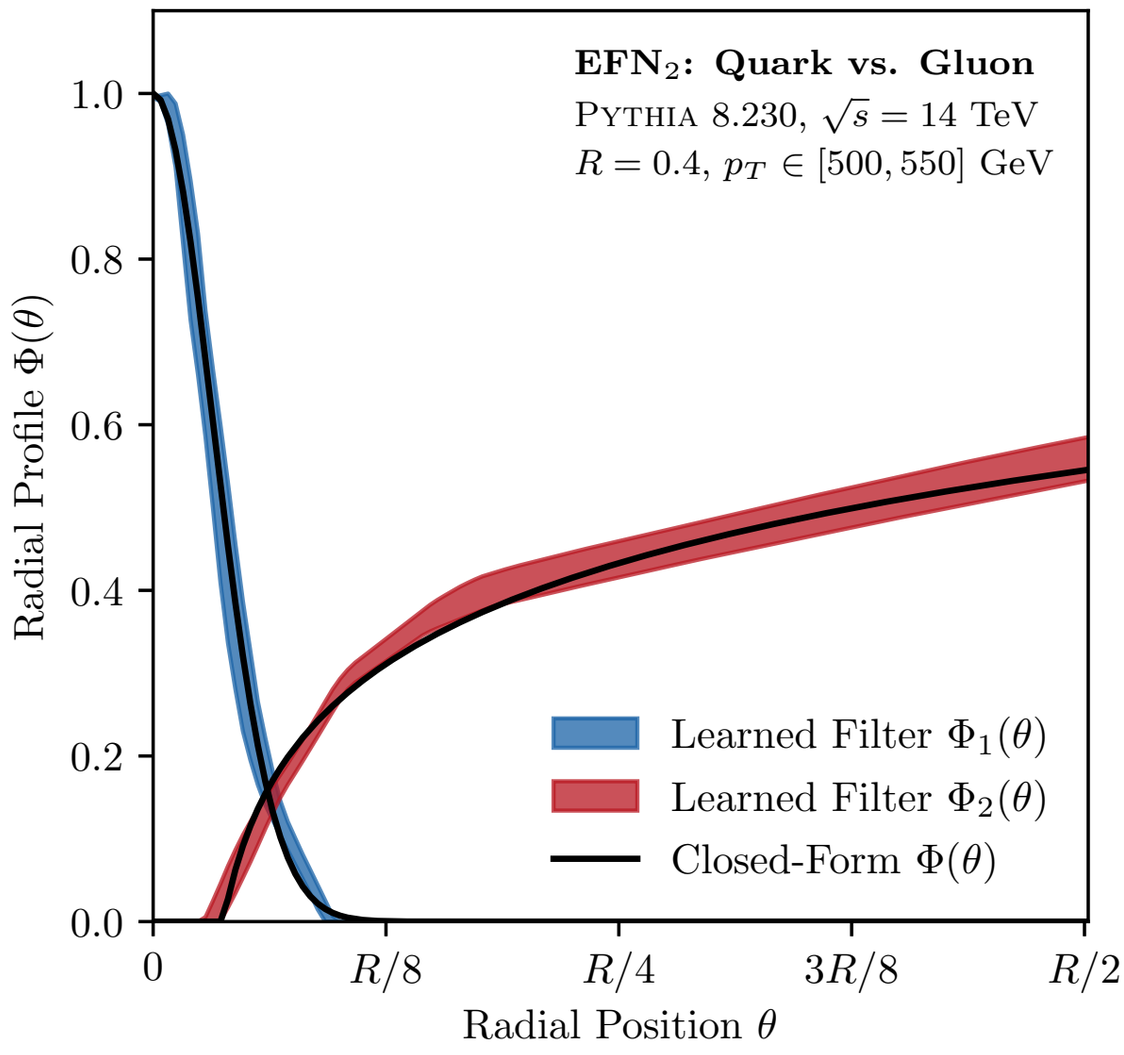
# Learning from the Machine




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

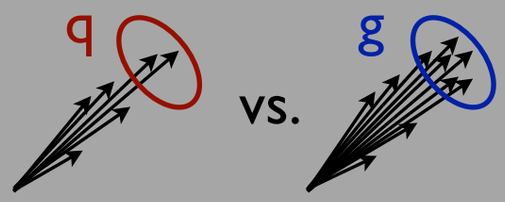
cf. Angularities:
$f(\theta) = \theta^\beta$




[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

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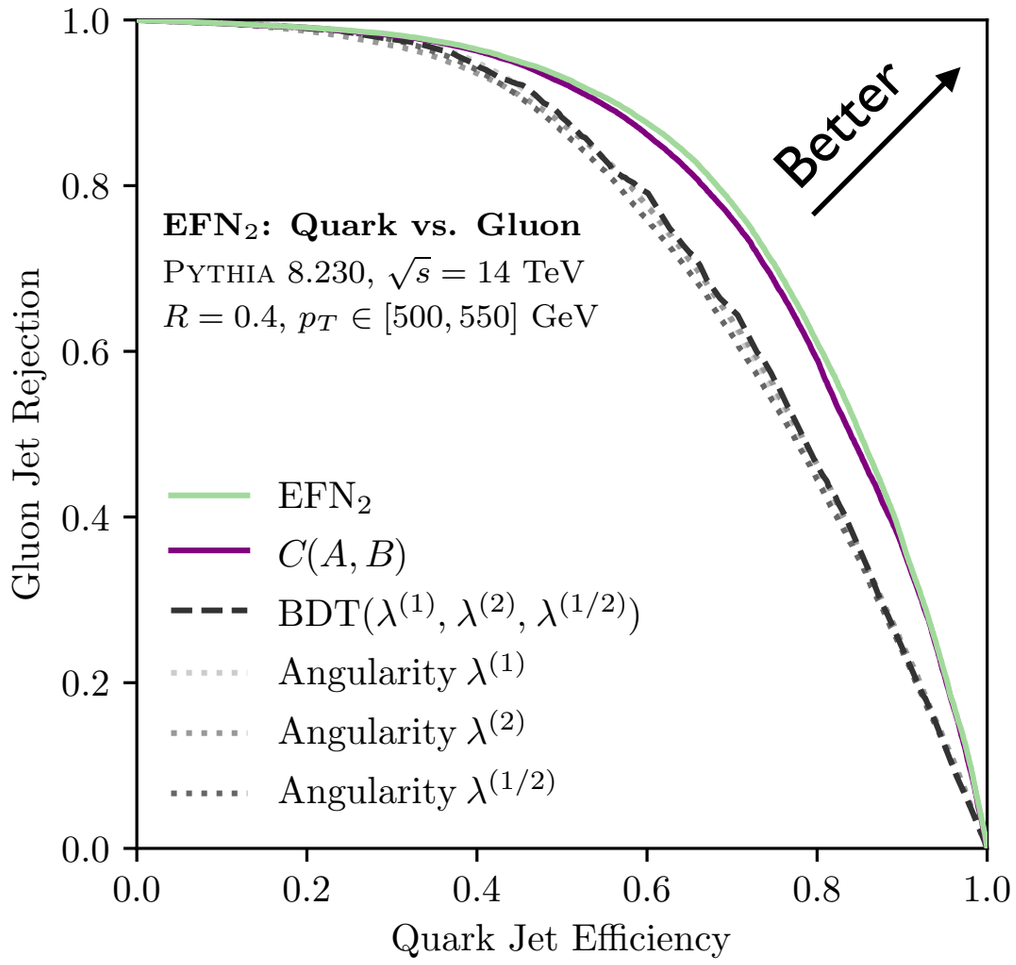
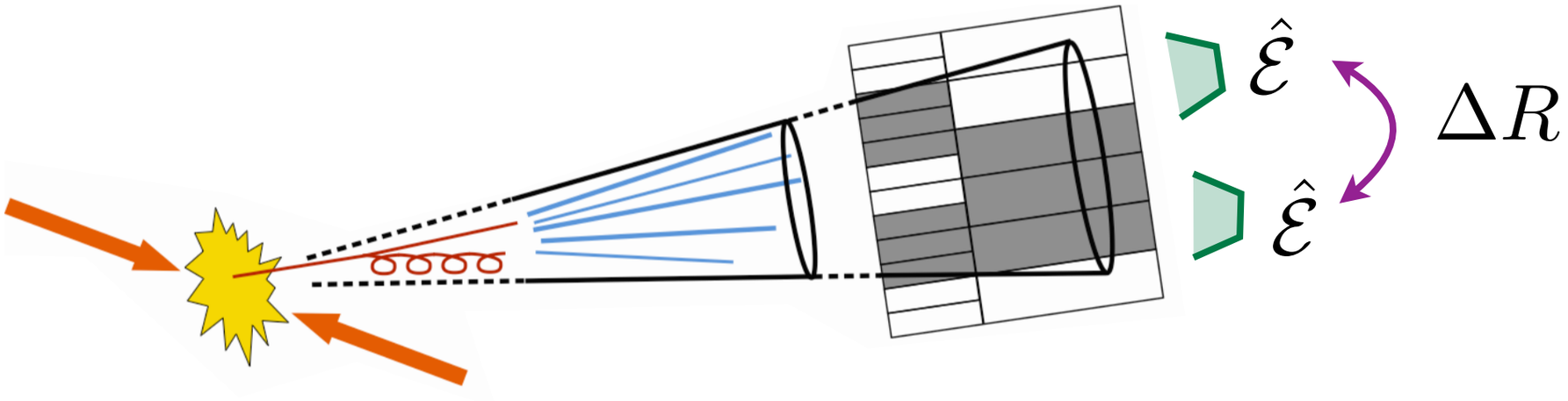



EFN outperformed a domain expert (i.e. me)

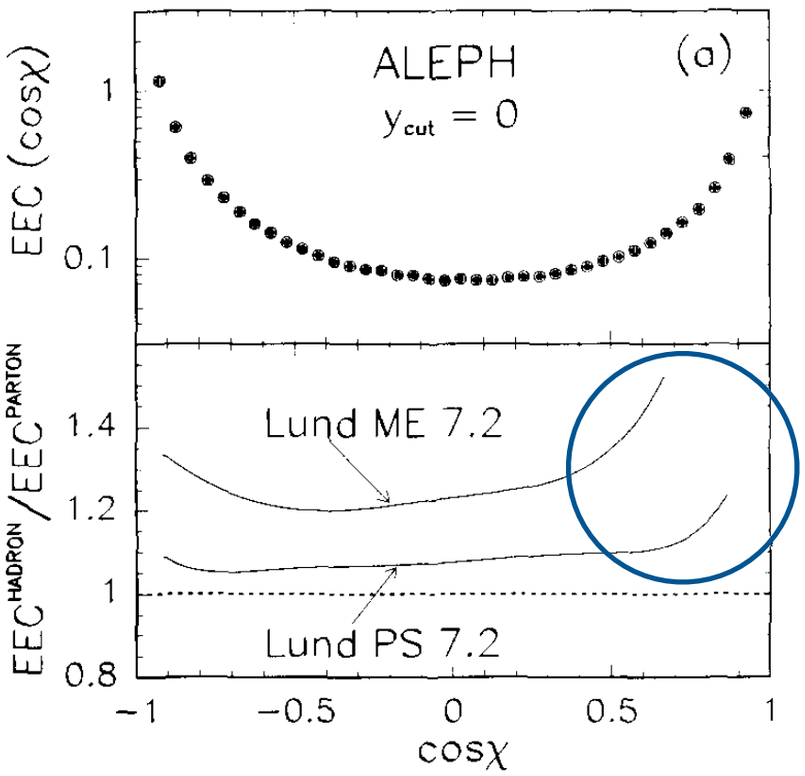
But we reverse engineered the machine (and learned something about QCD)

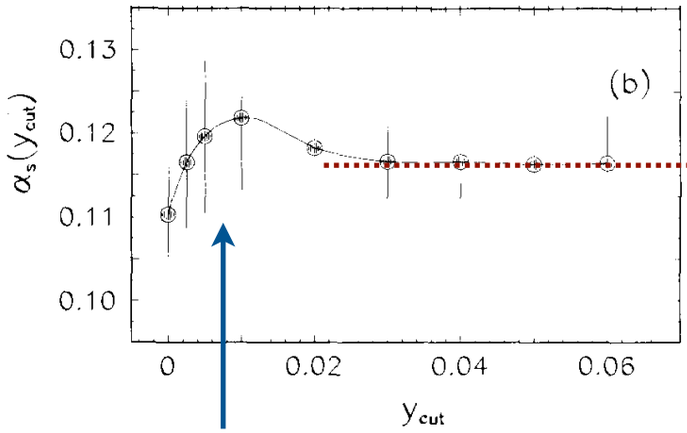
[Komiske, Metodiev, JDT, JHEP 2019;
cf. Larkoski, JDT, Waalewijn, JHEP 2014; using Berger, Kucs, Sterman, PRD 2003; Ellis, Vermilion, Walsh, Hornig, Lee, JHEP 2010]

# Energy-Energy Correlators




A long history in probing collinear dynamics of QCD



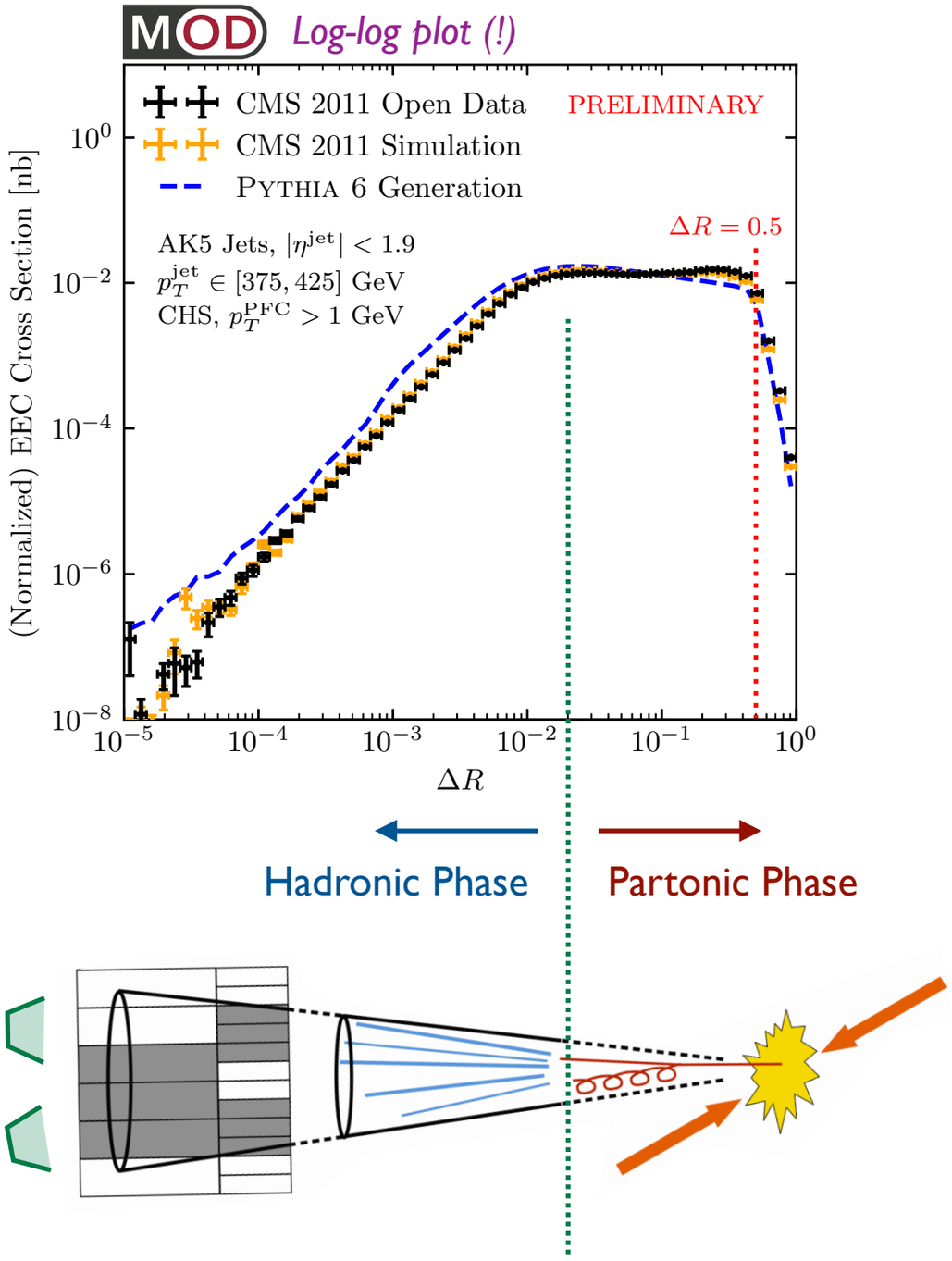




Extracting the strong coupling constant

Theoretical challenges with small angle (collinear) limit

[Basham, Brown, Ellis, Love, PRL 1978; ALEPH, PLB 1991; see Chen, Moult, Zhang, Zhu, PRD 2020]

# QCD Phase Transition in Jets?




Behind the scenes at BOOST 2019

**Jesse Thaler** July 24, 2019 at 2:01 PM

EE(E)C?

To: Ian Moult

Hi Ian,

I appreciate the provocative lunch! At some point, we should talk about what you might want to see measured on the CMS Open Data with respect to EE(E)C.

Cheers,
Jesse

**Jesse Thaler** July 24, 2019 at 10:16 PM

Preliminary EEC plot

To: Ian Moult, Cc: Patrick Komiske

Hi Ian,

Below is a preliminary EEC plot on the CMS Open Data, made by Patrick. (Strictly speaking, this is the pT-pT-Correlator...)

We do this within single jets in the pT range specified in the plot, and the dashed vertical red line is the jet radius (beyond which things don't really make sense).

[Komiske, Moult, JDT, et al., in progress; see talks by Moult, BOOST 2019, BOOST 2020]