

# The Geometry of Particle Collisions: Hidden in Plain Sight

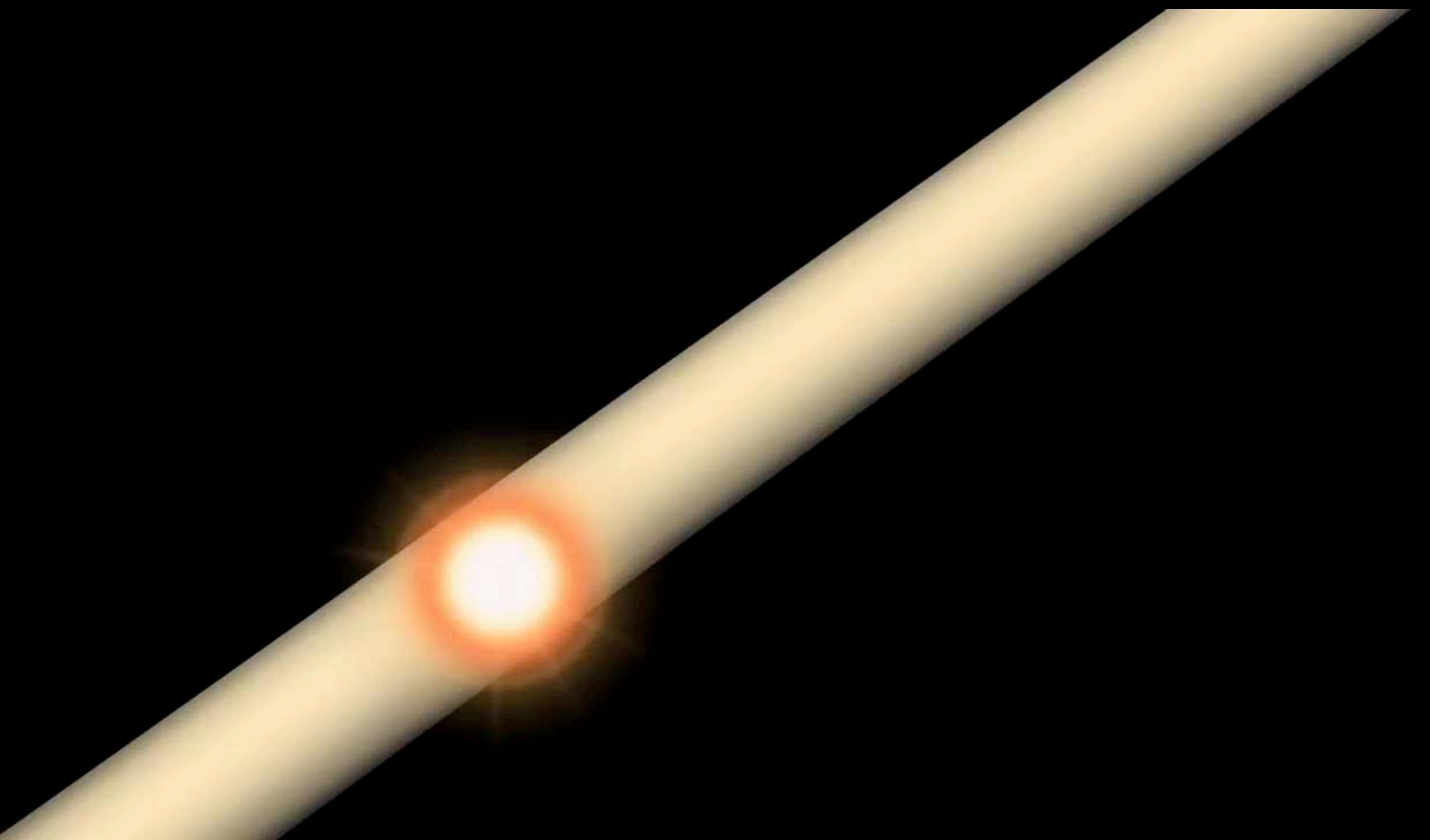
Jesse Thaler

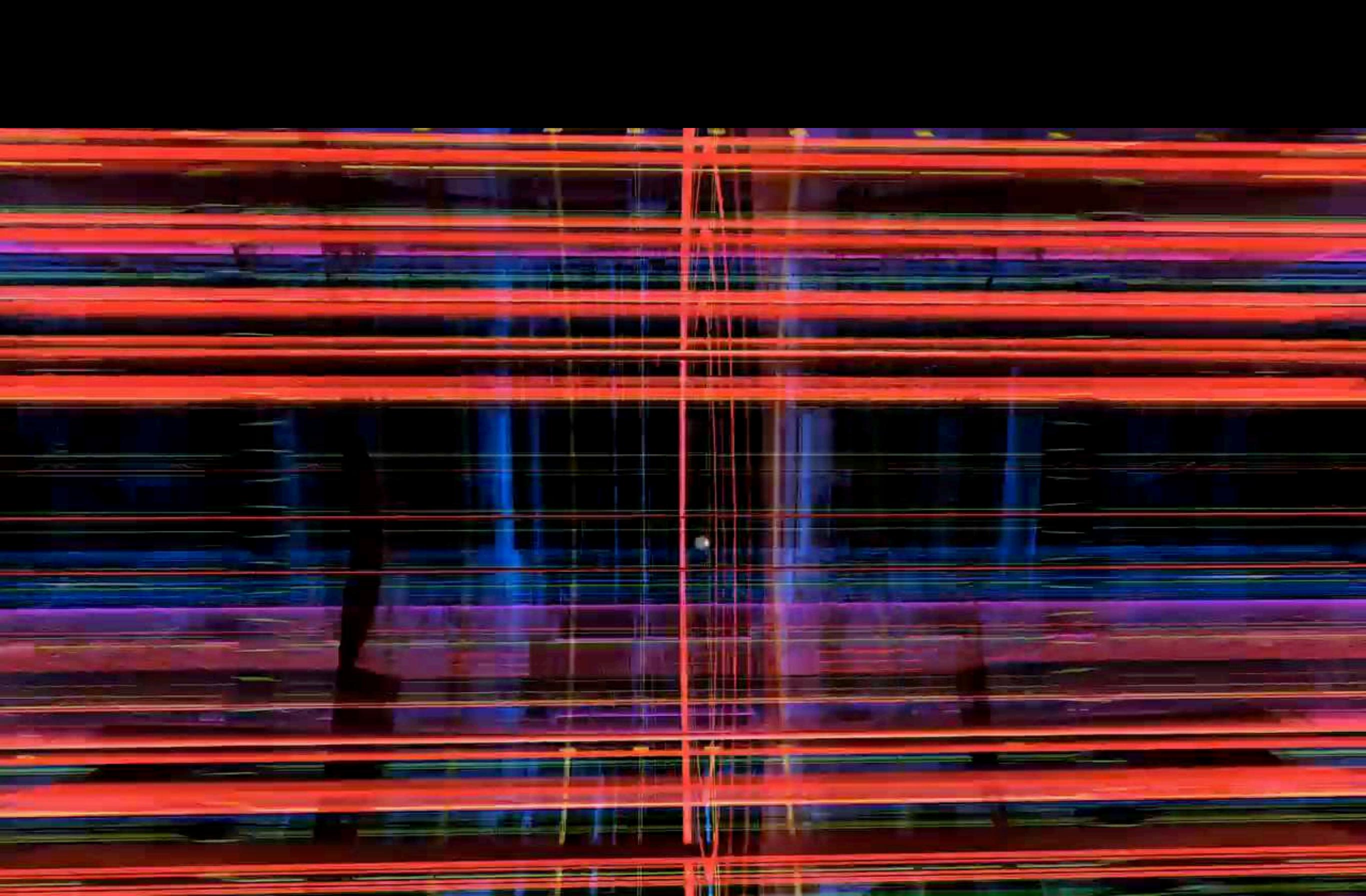


Physics Colloquium, Brandeis University — February 8, 2022

# The Geometry of Particle Collisions: Hidden in “Plane” Sight?

Physics Colloquium, Brandeis University — February 8, 2022



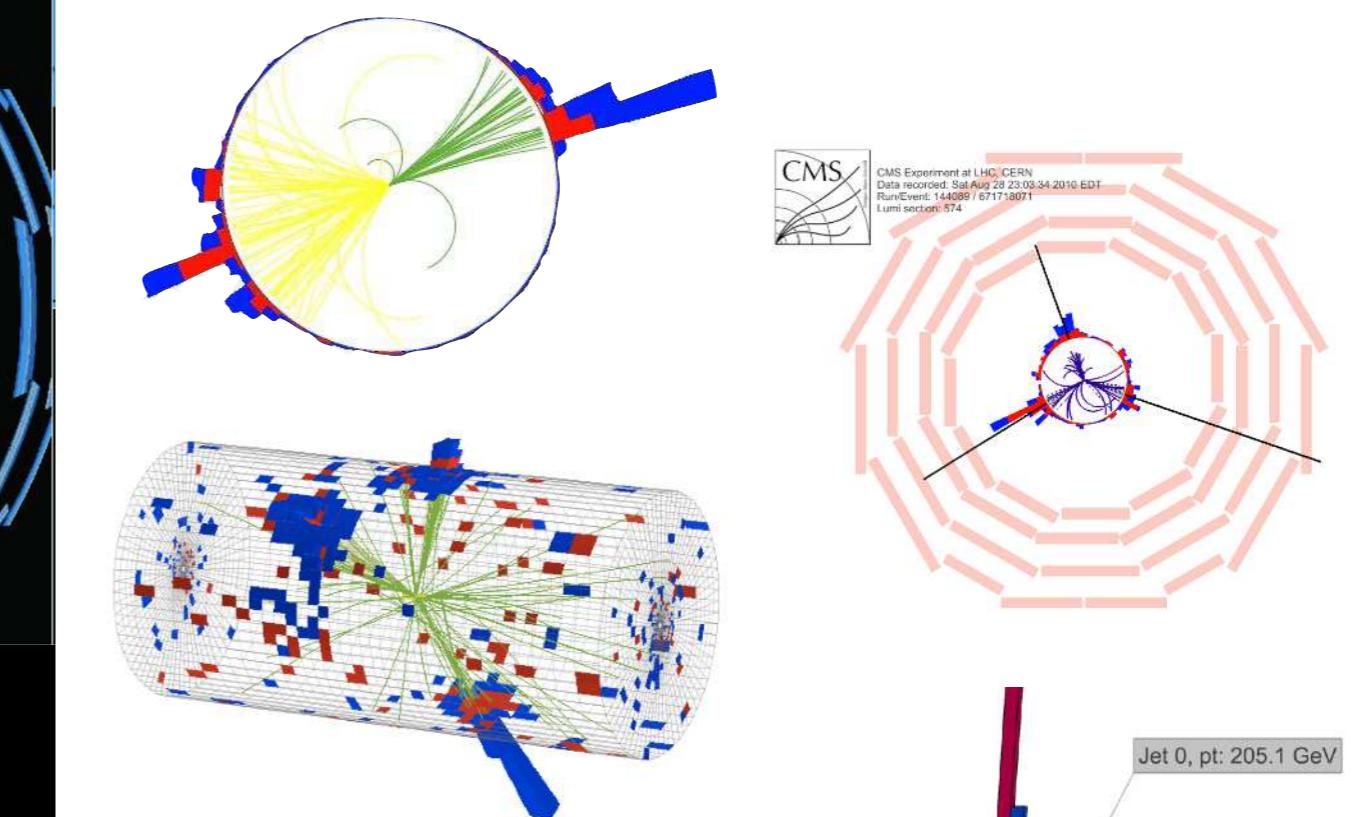
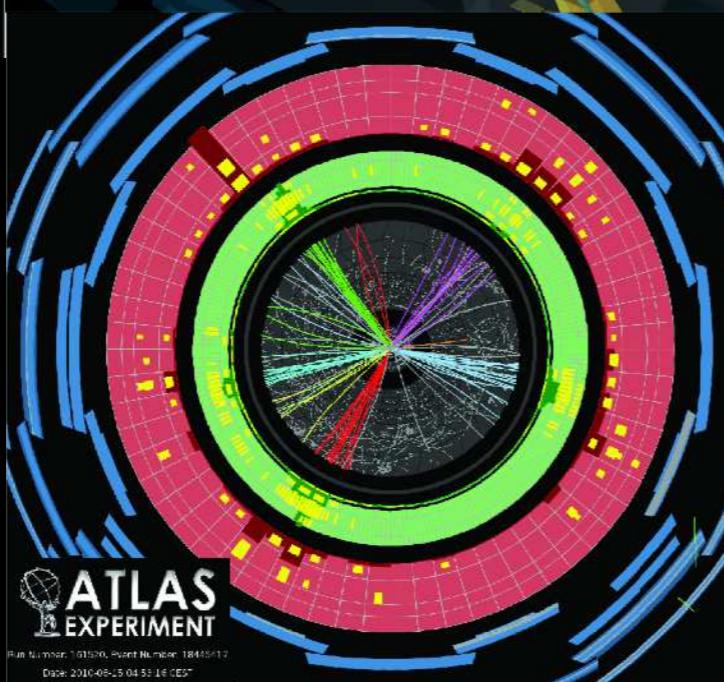
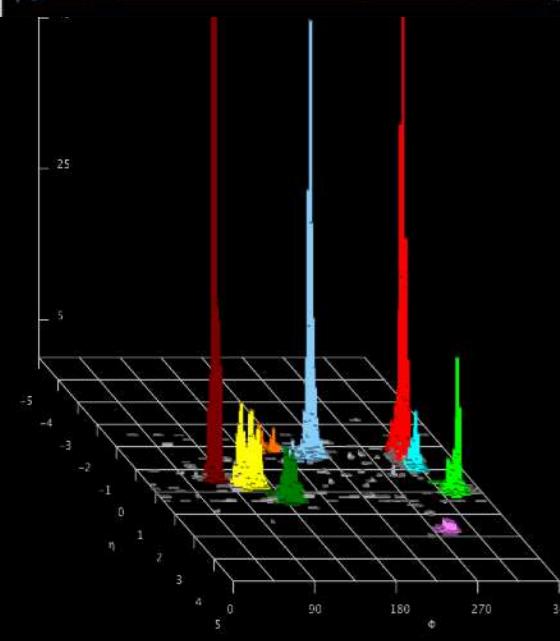
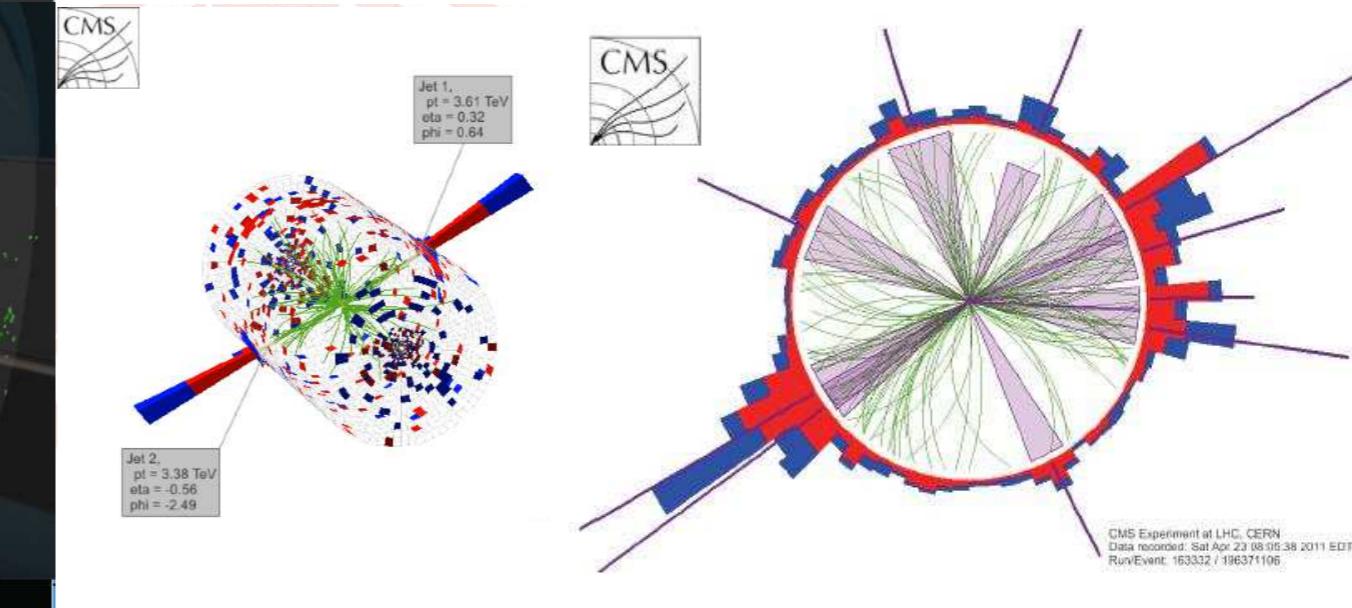
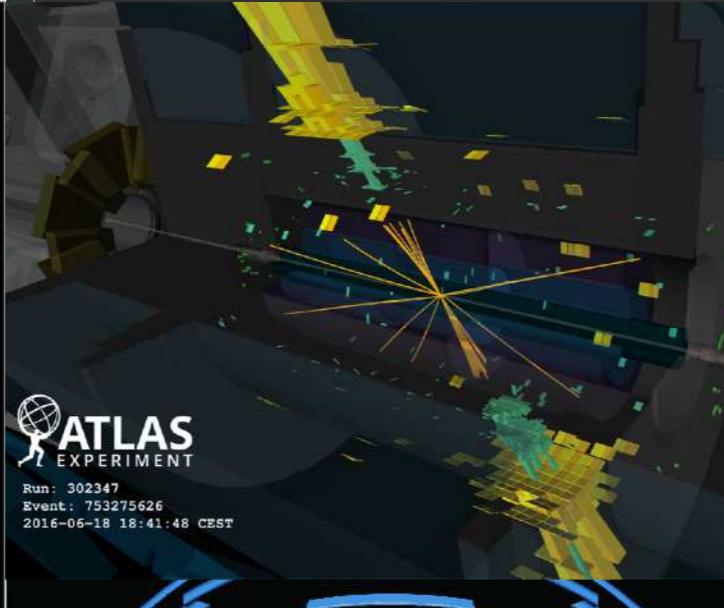
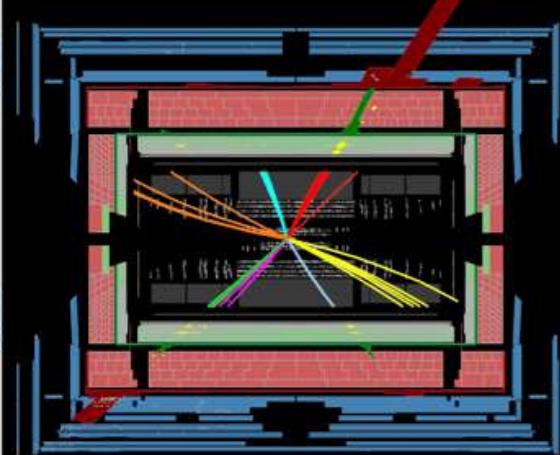




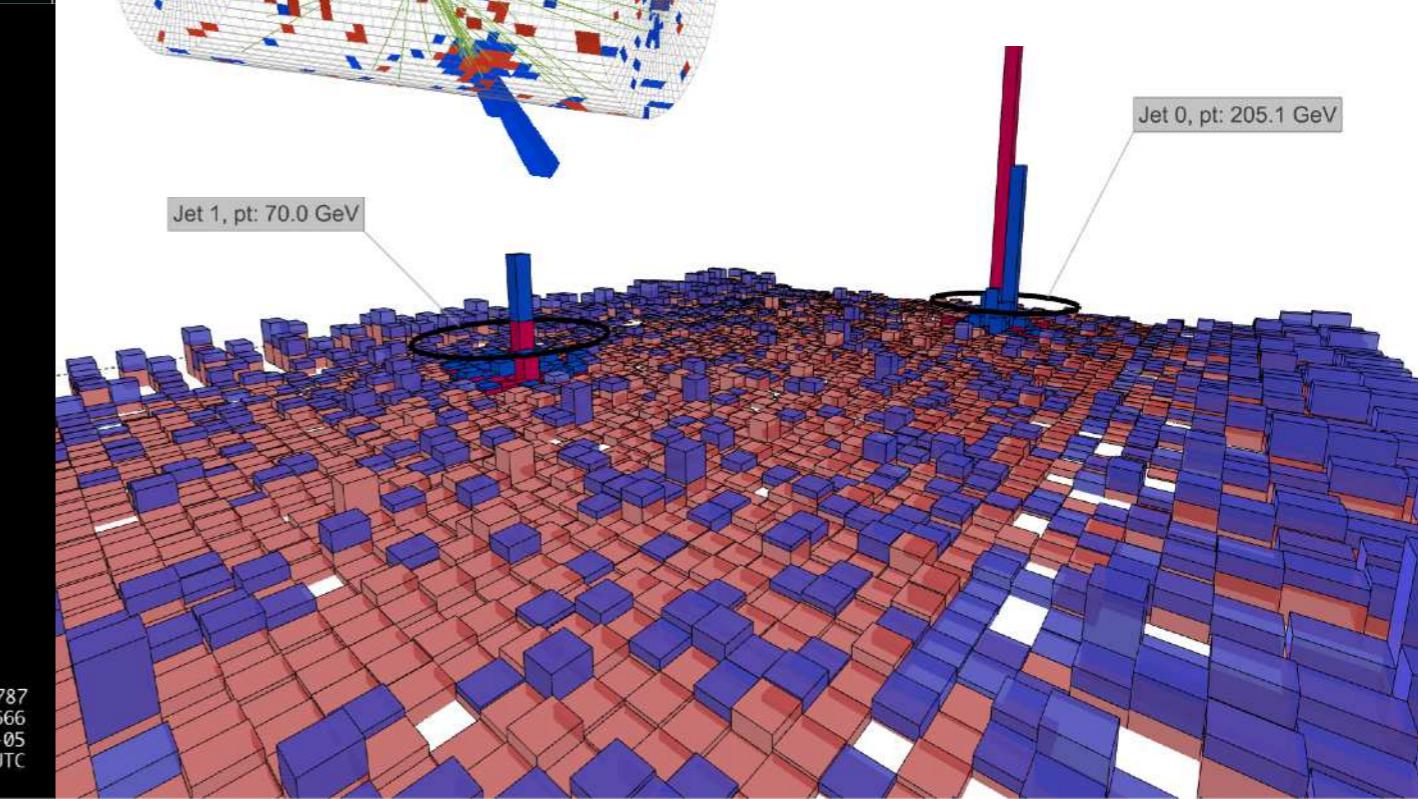
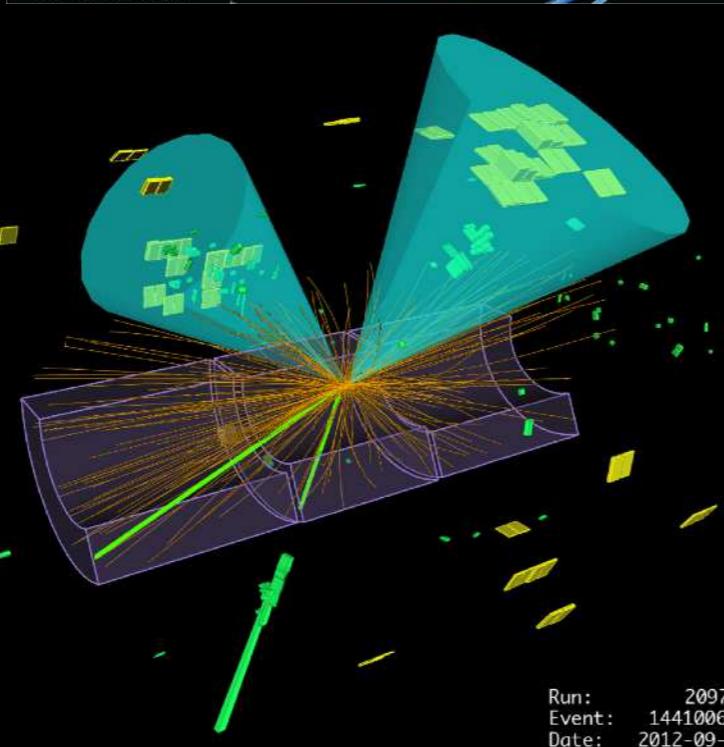
*“Jets” initiated by  
quarks & gluons in QCD*

Run Number: 159224, Event Number: 3533152

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

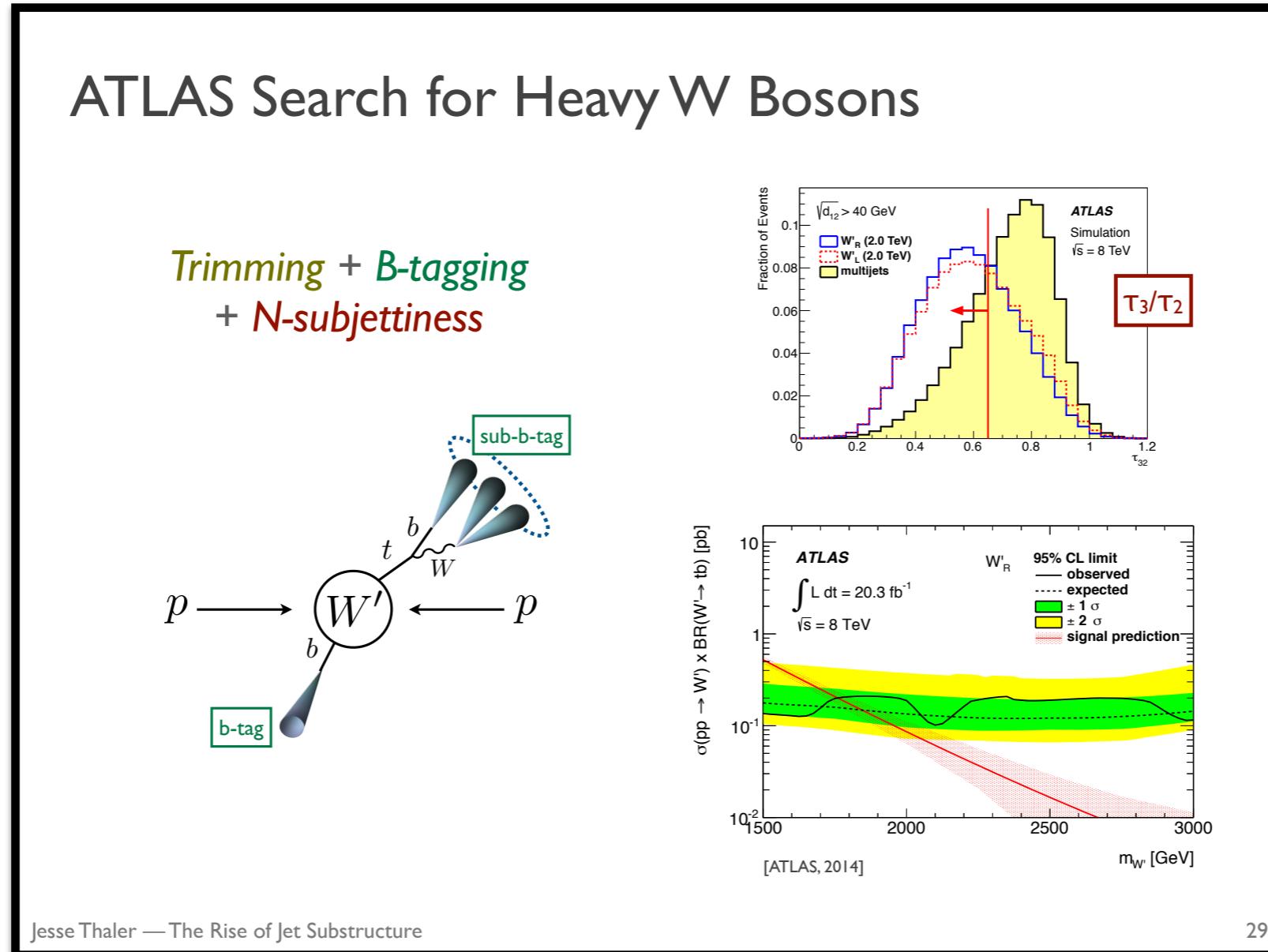


ATLAS  
EXPERIMENT  
<http://atlas.ch>



# 2015 Brandeis Colloquium

## *The Rise of Jet Substructure in Searching for New Phenomena at Colliders*



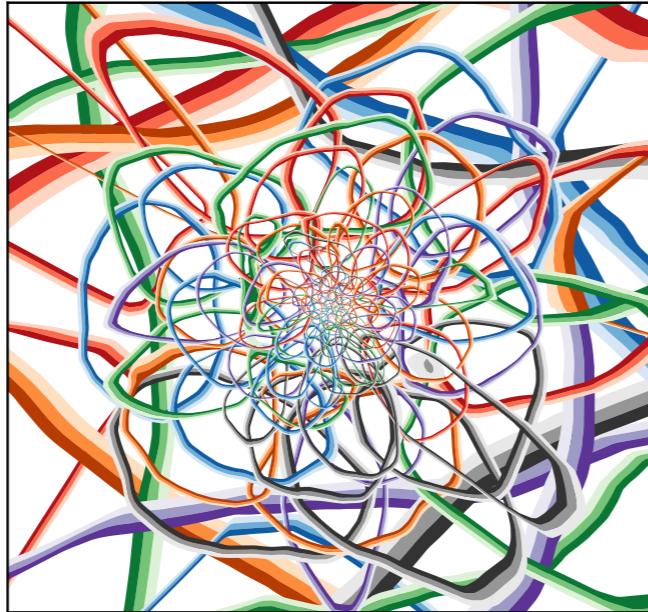
**“Why is N-subjettiness the preferred analysis strategy?”**

# 2019 Brandeis Seminar

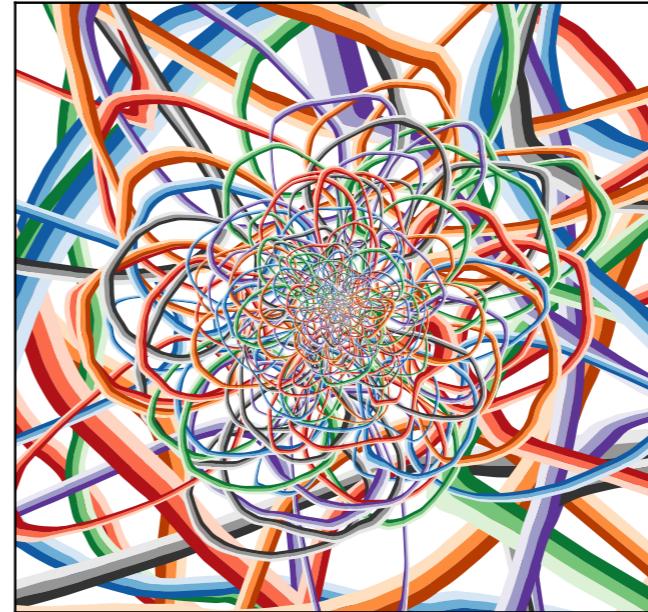
## *The Rise of Machine Learning for Deciphering Collider Data*

### Psychedelic Network Visualization

Latent Dimension 128



Latent Dimension 256



*Collinear singularity of QCD!*

Jesse Thaler (MIT) — Collision Course: Particle Physics as a Machine-Learning Testbed

43

**“Can we ever hope to understand what the machine is learning?”**

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

“eye-phi”



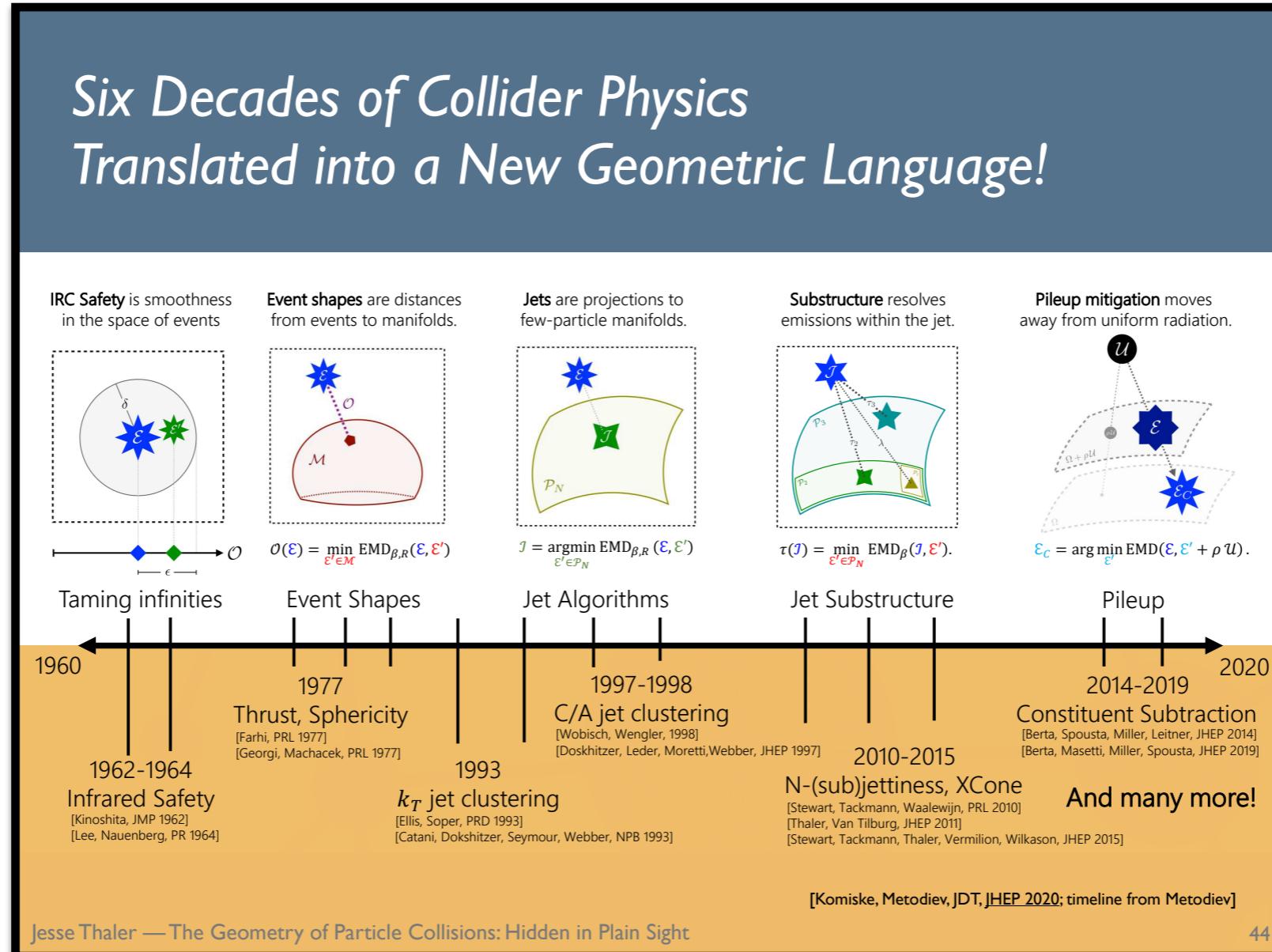
*Advance physics knowledge — from the smallest building blocks of nature  
to the largest structures in the universe — and galvanize AI research innovation*



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

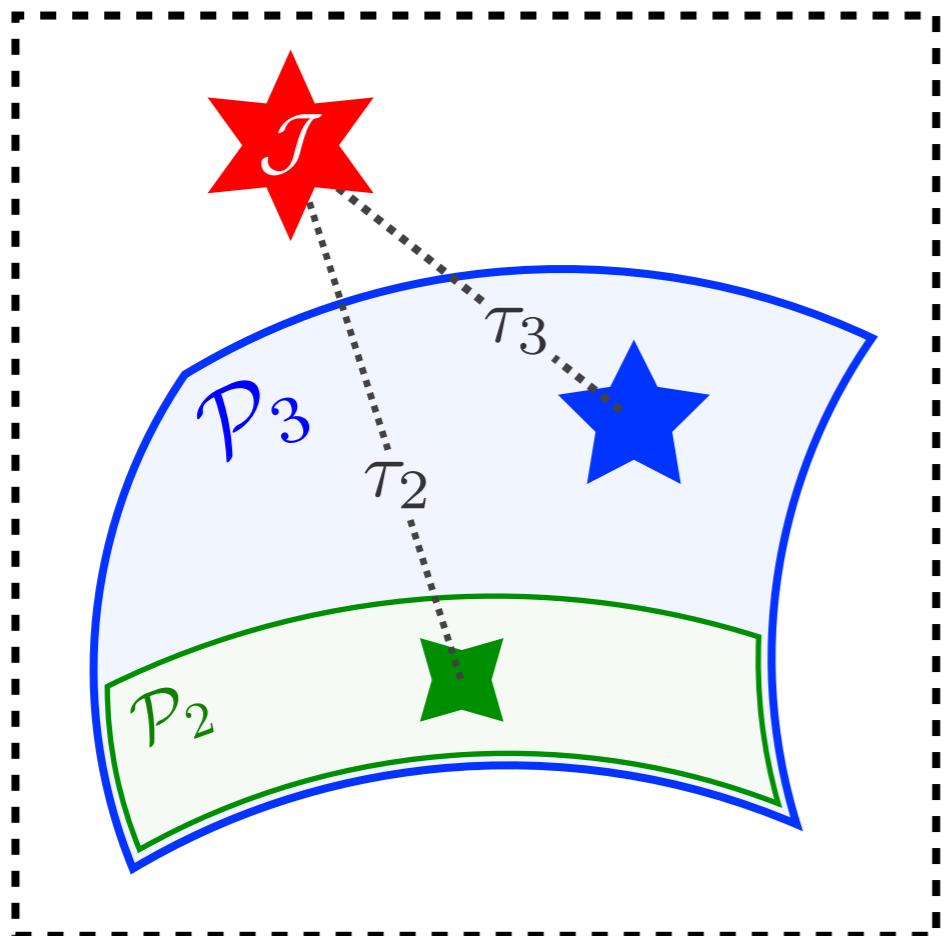
# 2022 Brandeis Colloquium

*The more things change, the more they stay the same...*



*Physics intelligence translated into language of artificial intelligence*

# Today's Punchline



N-subjettiness is a natural  
“geometric” object defined  
on the “space” of collider events

Suggests exciting applications of  
optimal transport theory  
for the LHC and beyond

Optimal transport for new sampling algorithms and efficient generative models

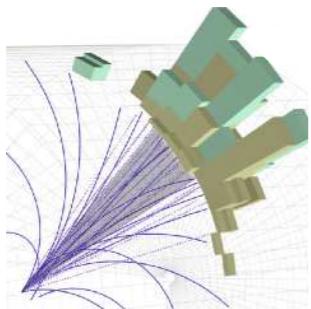
January 25, 2022

Tyler Maunu, Brandeis University

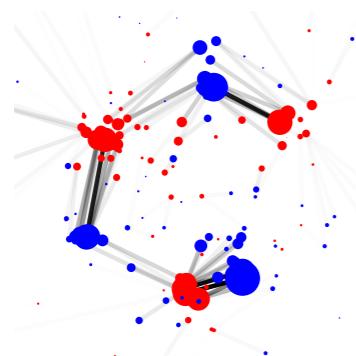
Host: Aram Apyan

Coincidence?  
I think not.

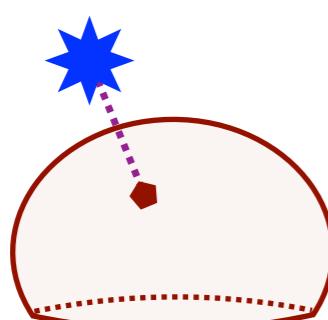
# Outline



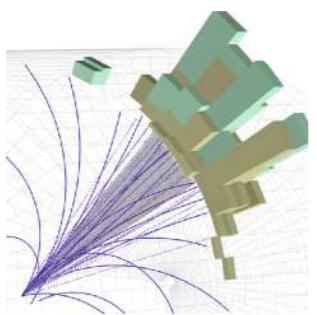
Going with the (Energy) Flow



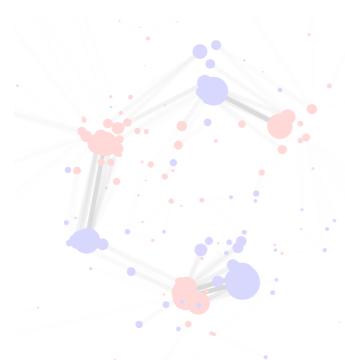
The Energy Mover's Distance



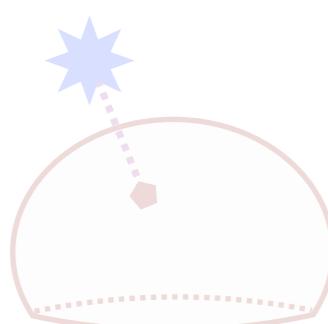
Revealing a Hidden Geometry



## Going with the (Energy) Flow



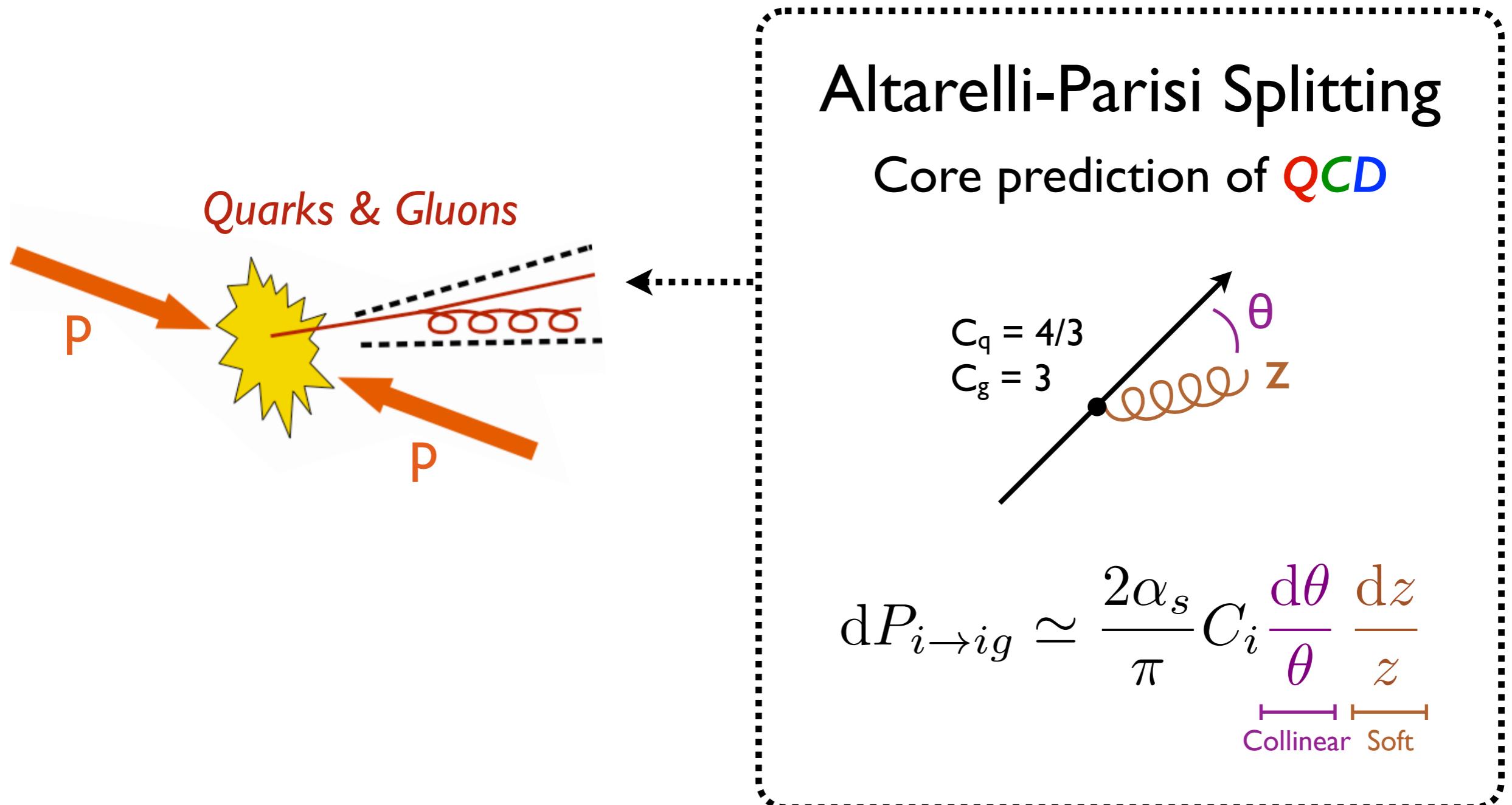
## The Energy Mover's Distance



## Revealing a Hidden Geometry

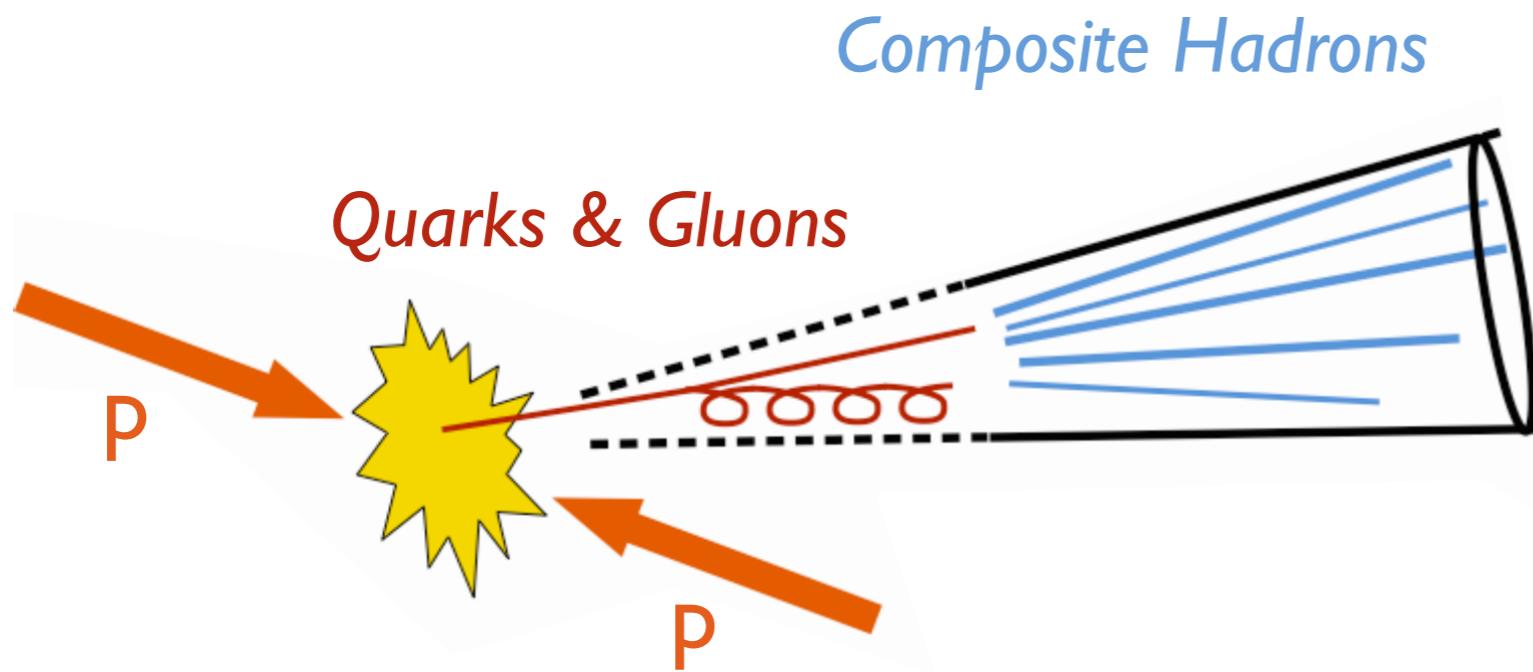
# Introducing Energy Flow

Respects *infrared and collinear safety*



# Introducing Energy Flow

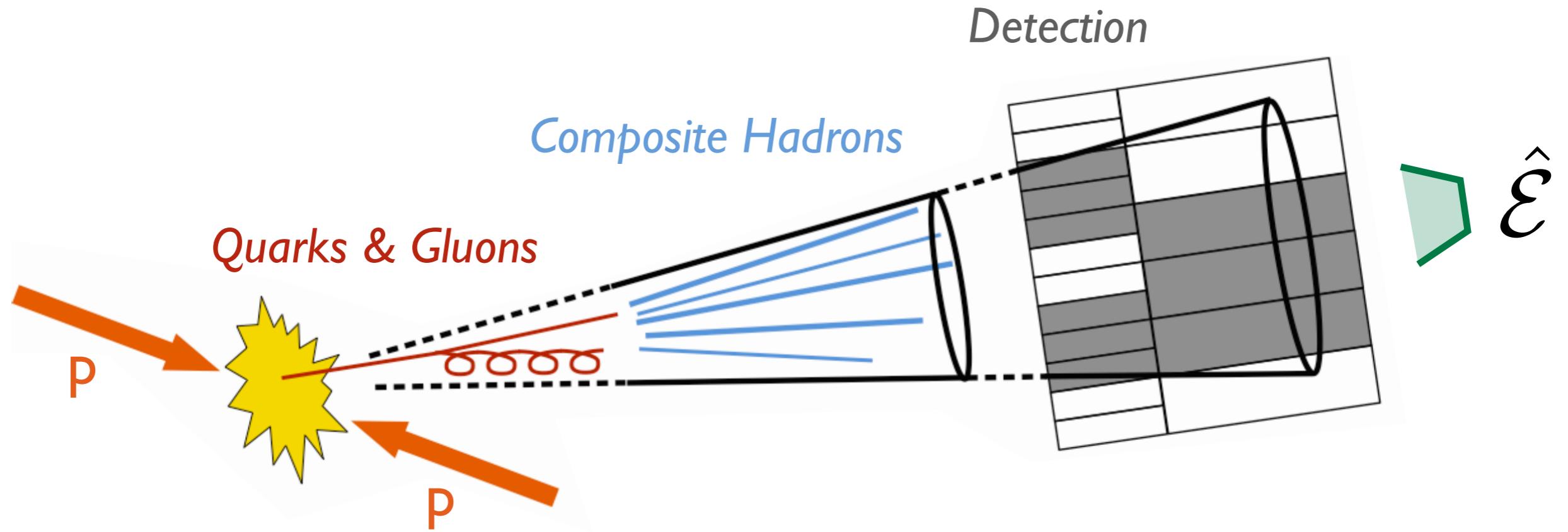
Respects *infrared and collinear safety*



# Introducing Energy Flow

Respects *infrared and collinear safety*

Theory

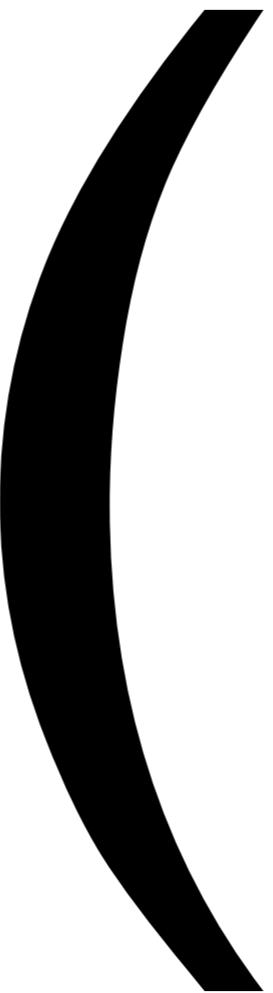


*Energy Flow:*

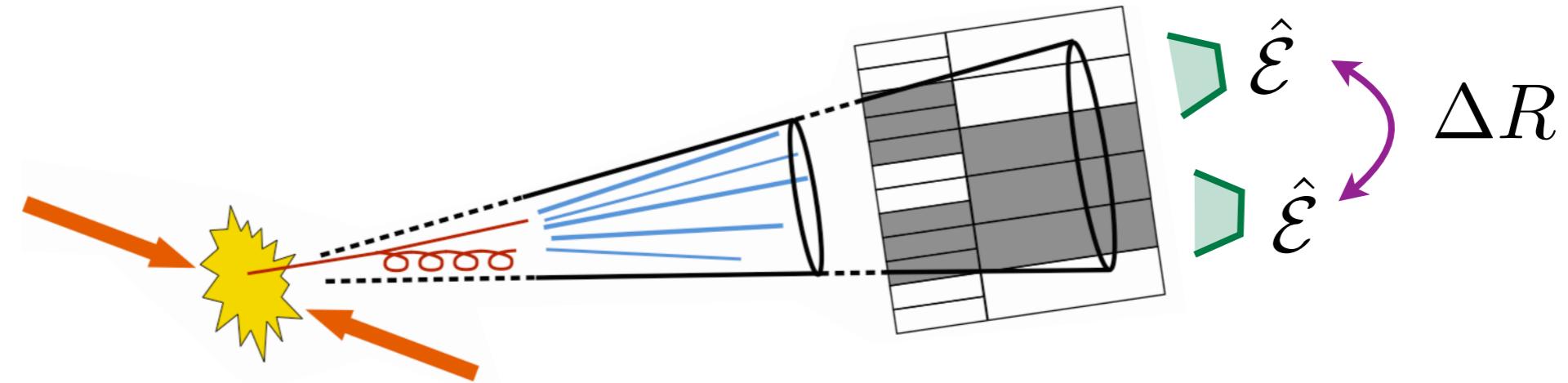
Robust to hadronization and detector effects

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

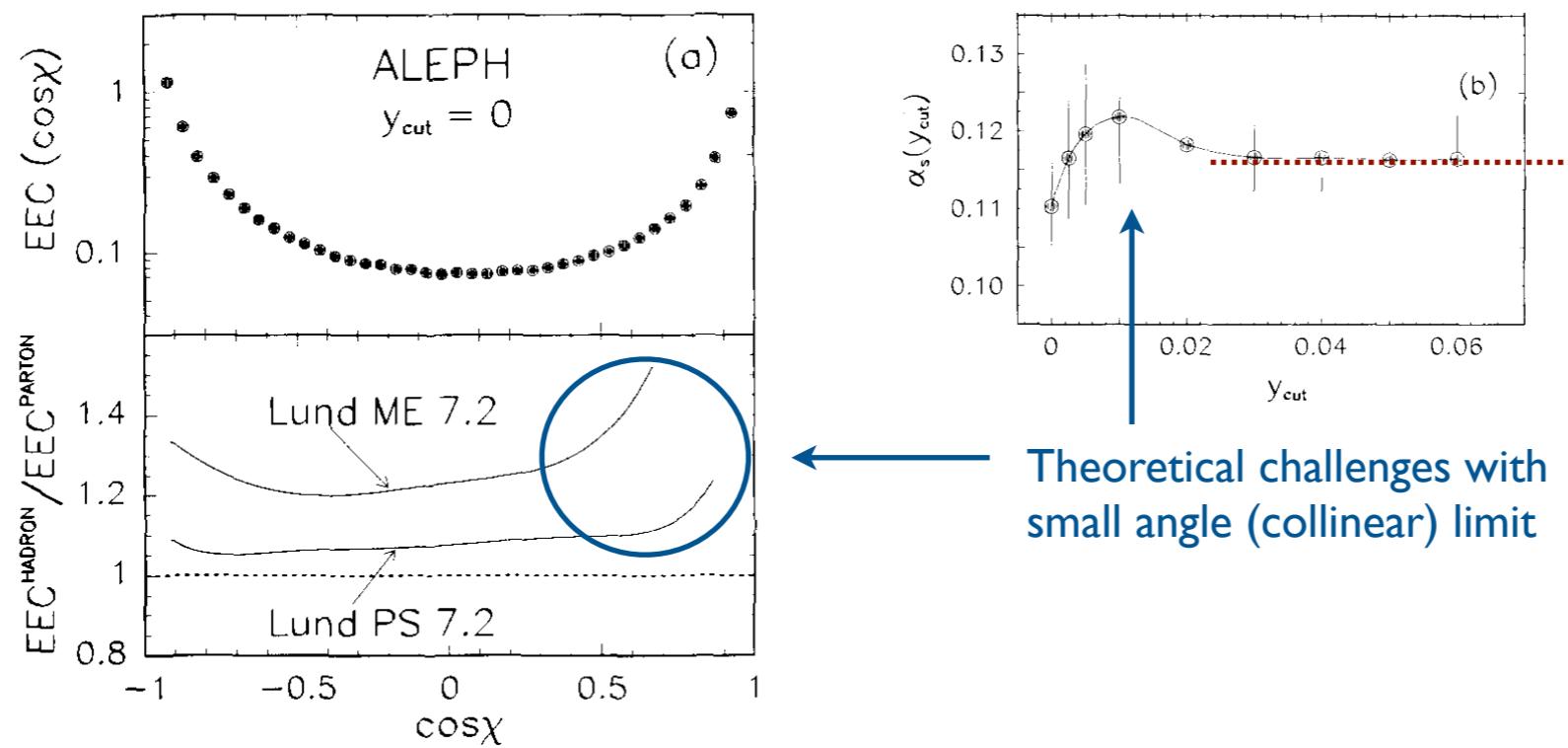
[see e.g. Sveshnikov, Tkachov, [PLB 1996](#); Hofman, Maldacena, [JHEP 2008](#); Mateu, Stewart, [JDT, PRD 2013](#); Belitsky, Hohenegger, Korchemsky, Sokatchev, Zhiboedov, [PRL 2014](#); Chen, Moult, Zhang, Zhu, [PRD 2020](#)]



# Energy-Energy Correlators

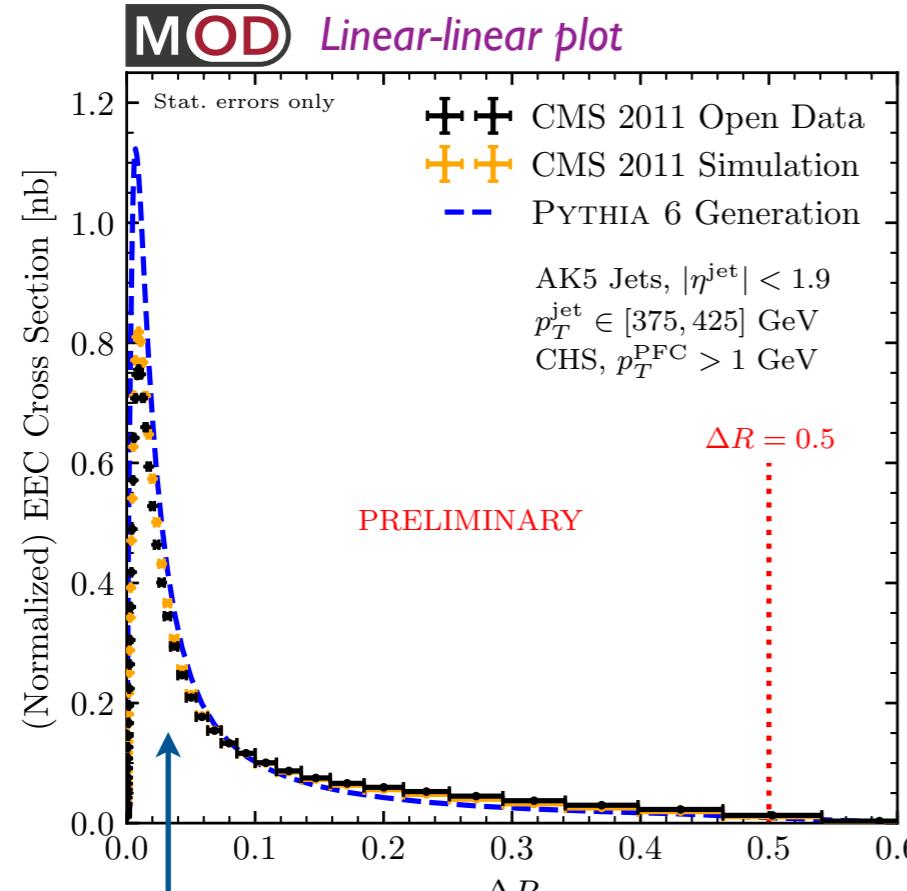


A long history in probing collinear dynamics of QCD



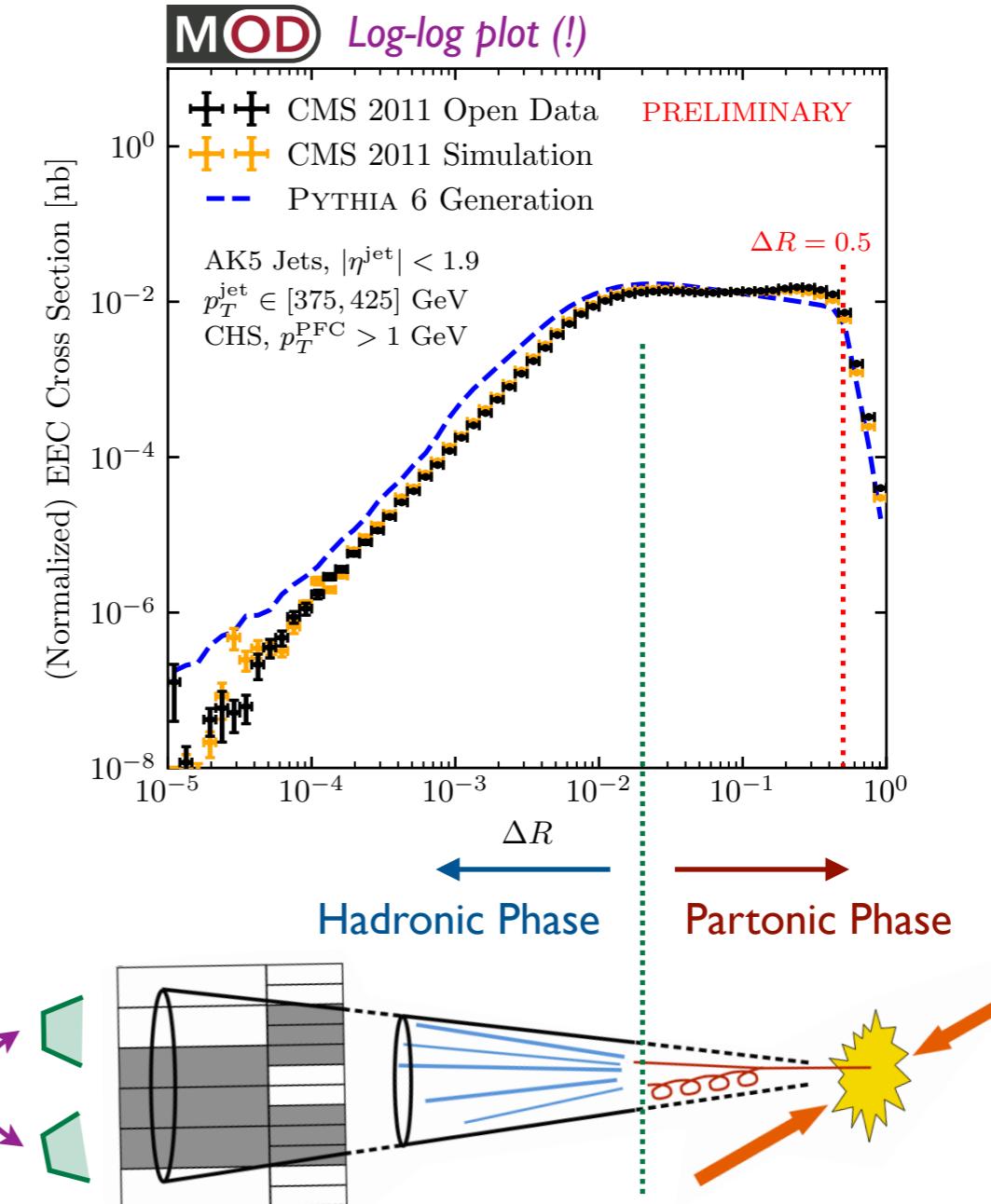
[Basham, Brown, Ellis, Love, [PRL 1978](#); ALEPH, [PLB 1991](#); see Chen, Moult, Zhang, Zhu, [PRD 2020](#)]

# QCD Phase Transition in Jets?



Are we learning something about small angle limit of QCD?

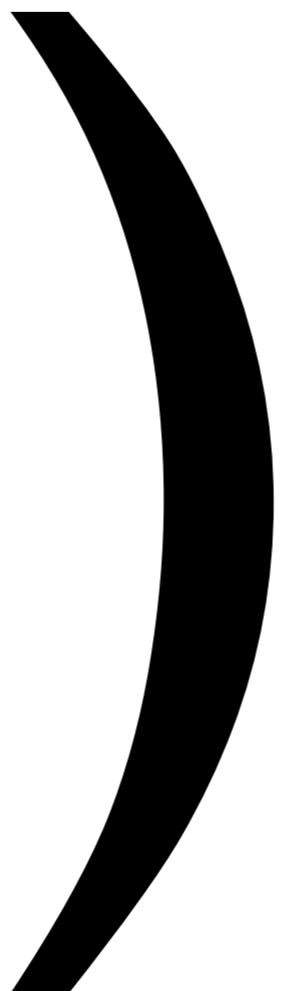
First Jet EEC Plot from the LHC (!)



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

This music video images the  
real-time confinement transition in QCD  
at the shortest time scale  
in real LHC data  
from free hadrons at low energies (small angles)  
to interacting quarks and gluons with non-trivial correlations  
at high energies (large angles).

[[Zhu on YouTube](#)]



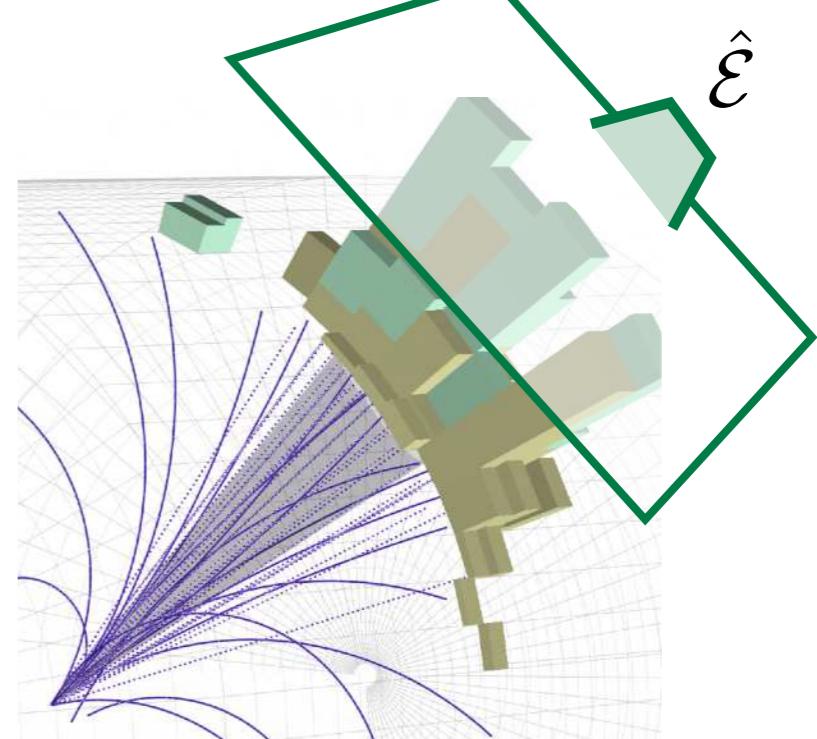
# Jets as Weighted Point Clouds

- Energy-Weighted Directions

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

↑      |  
Energy      Direction

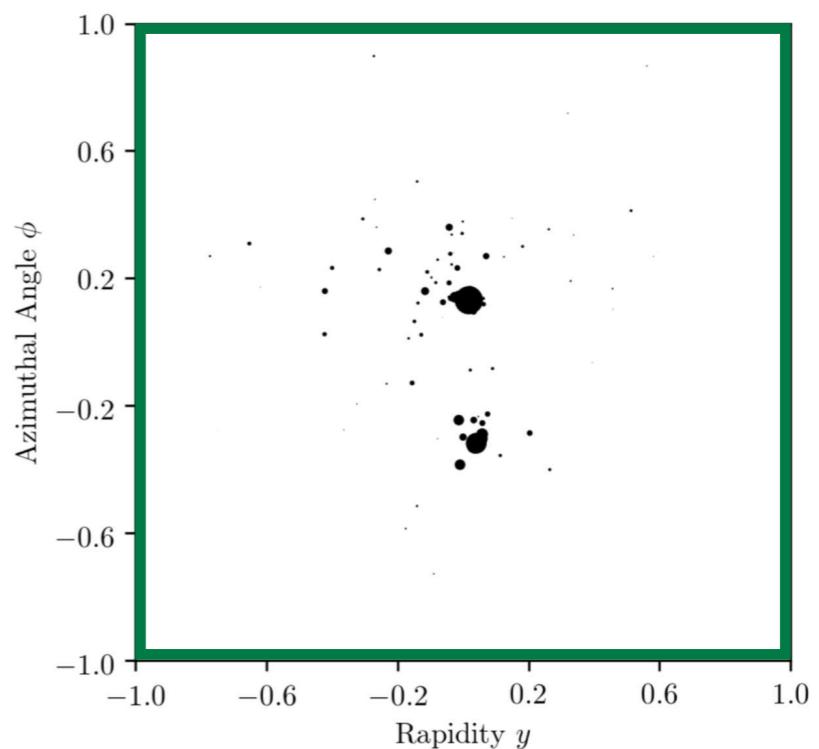
(suppressing “unsafe” charge/flavor information)

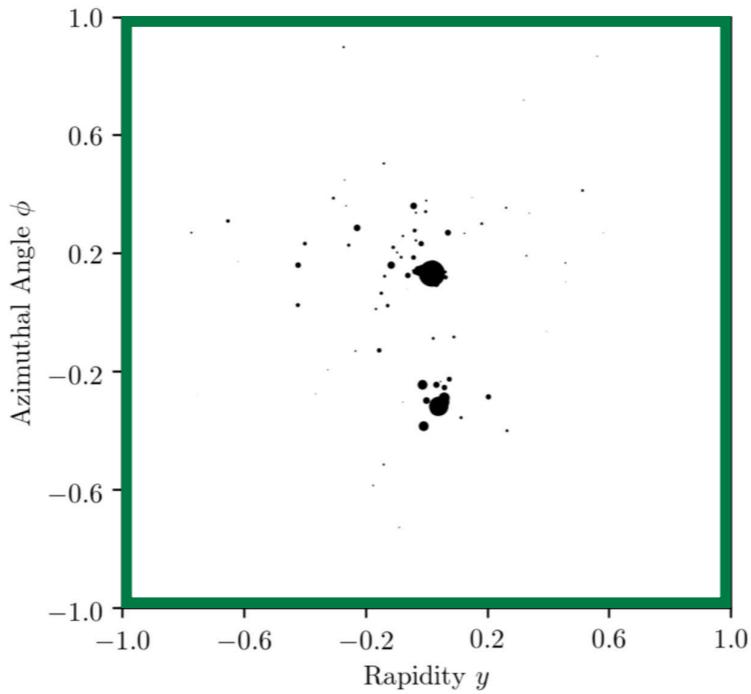


- Equivalently: Energy Density

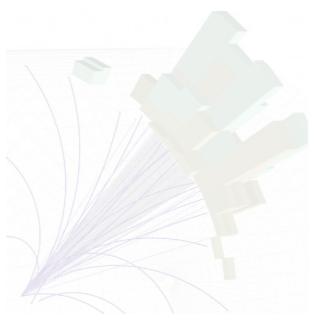
$$\rho(\hat{n}) = \sum_{i \in \mathcal{J}} E_i \delta^{(2)}(\hat{n} - \hat{n}_i)$$

↑      ↑  
Energy      Direction

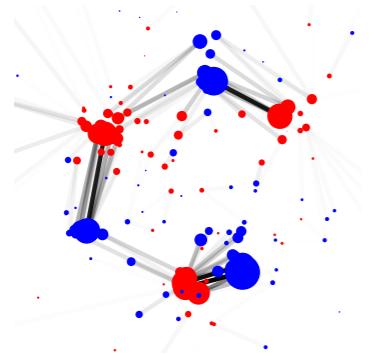




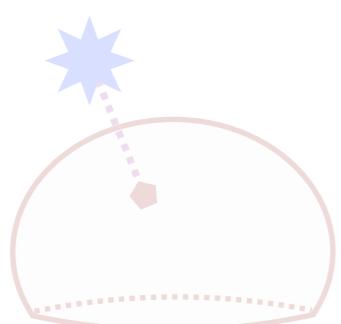
*When restricted to IRC safe information,  
jets/events are naturally represented  
as **energy densities***



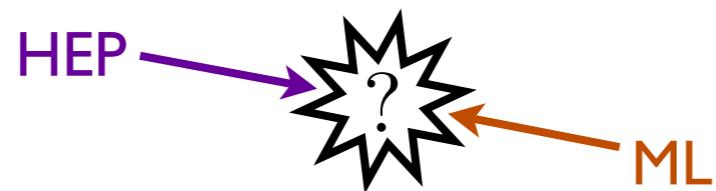
## Going with the (Energy) Flow



## The Energy Mover's Distance



## Revealing a Hidden Geometry



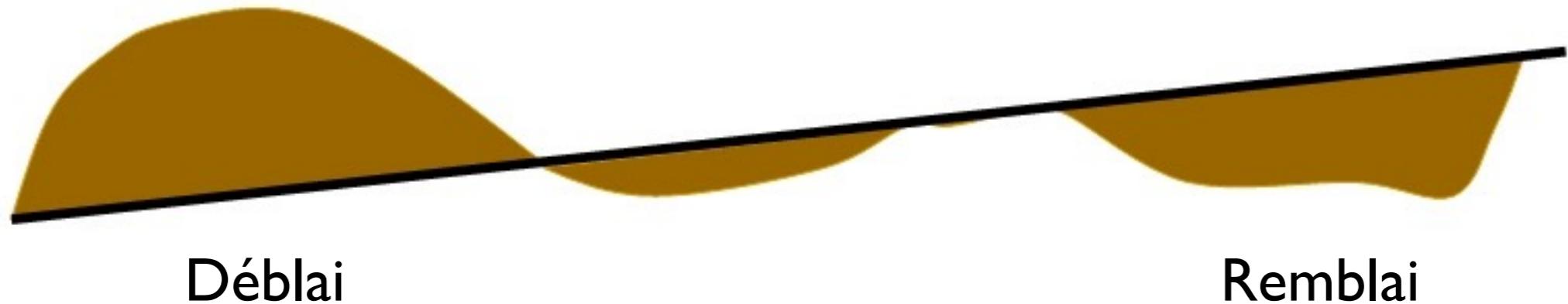
*If you ask your local computational geometry  
expert how to process densities...*

# The Earth Mover's Distance

## Optimal Transport:

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

Minimum “work” (stuff  $\times$  distance) to make one distribution look like another distribution



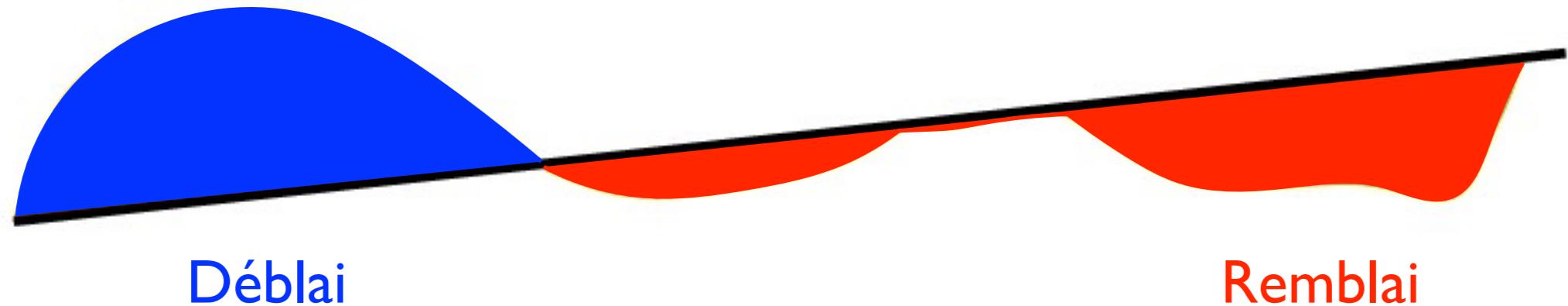
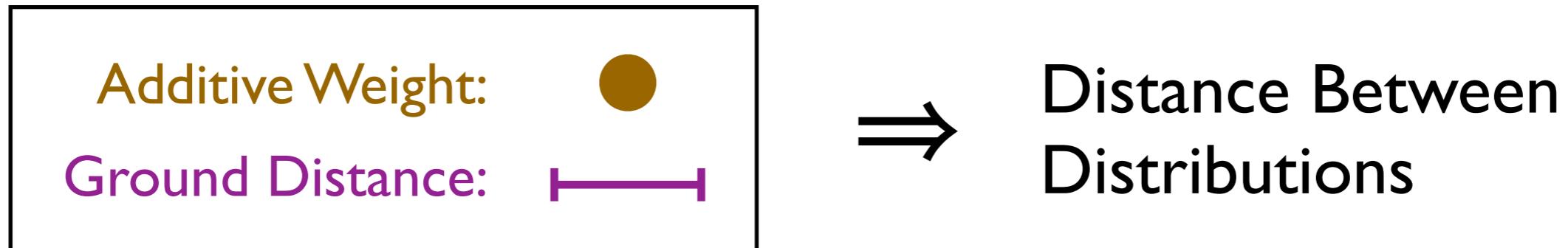
[h/t Niles-Weed, [ML4Jets 2020](#); Monge, 1781; Kantorovich, 1939; Vaserštejn, 1969; [Wikipedia](#)]

# The Earth Mover's Distance

Optimal Transport:

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

Minimum “work” (**stuff** × **distance**) to make  
**one distribution** look like **another distribution**



[h/t Niles-Weed, [ML4Jets 2020](#); Monge, 1781; Kantorovich, 1939; Vaserštejn, 1969; [Wikipedia](#)]

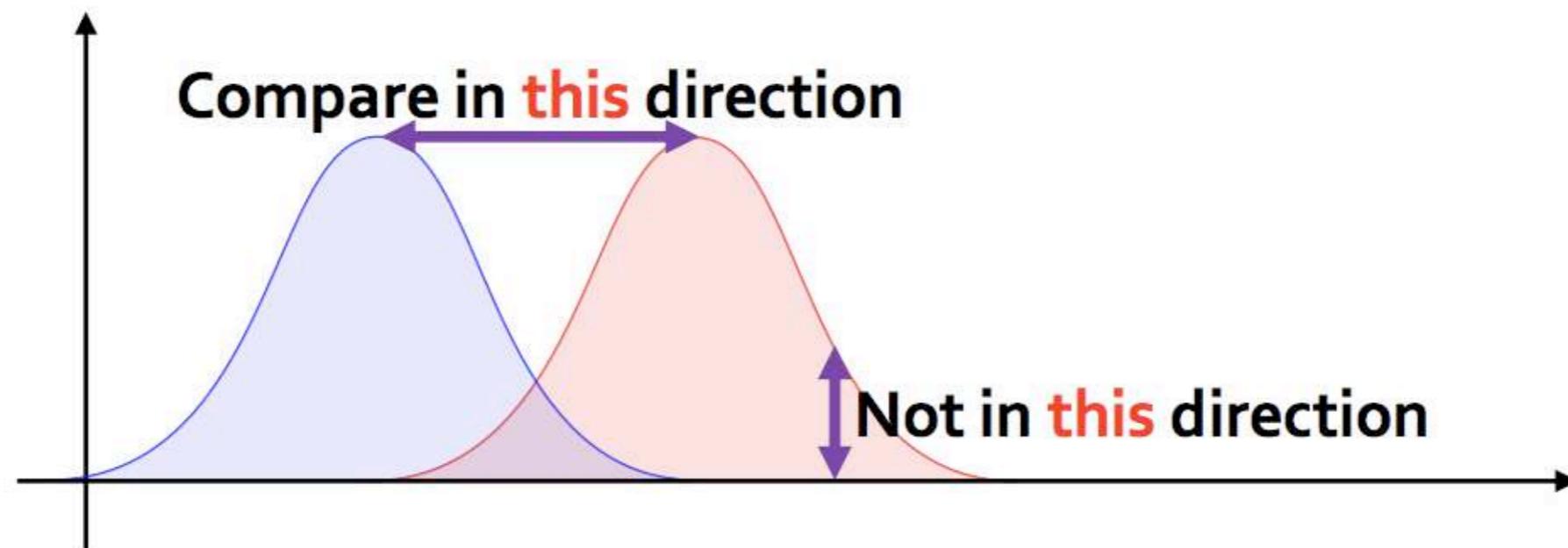
# The Earth Mover's Distance

## Optimal Transport:

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

Minimum “work” (**stuff  $\times$  distance**) to make  
**one distribution** look like **another distribution**

“Horizontal” comparison (EMD) yields better  
dynamic range than “vertical” comparison (e.g. KL)

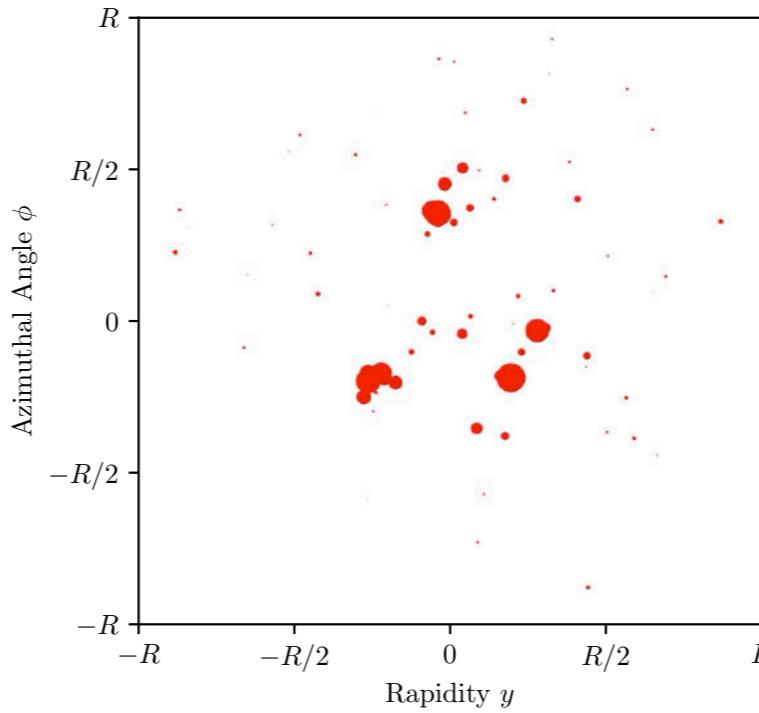


[figure from Kun, [Math n Programming](#)]

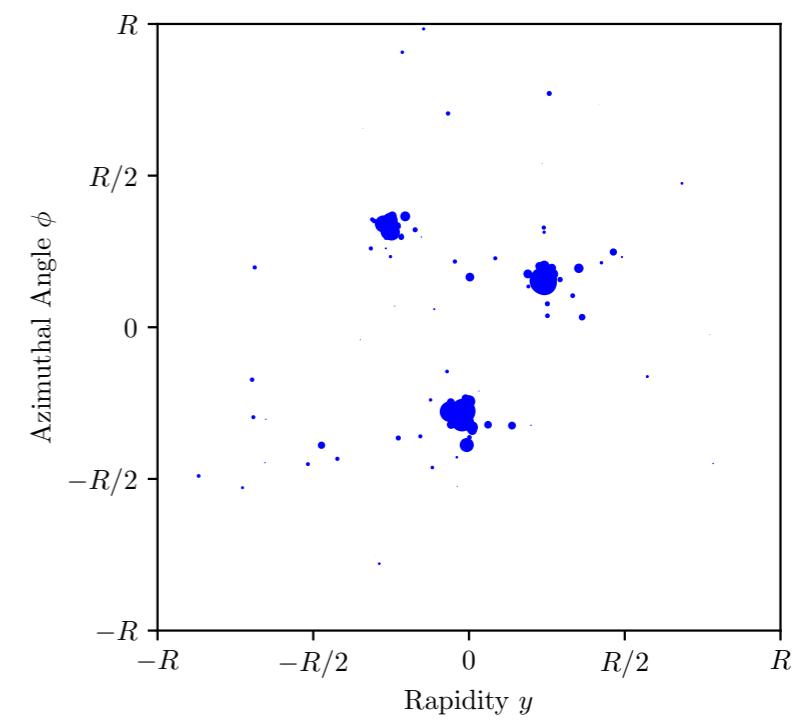
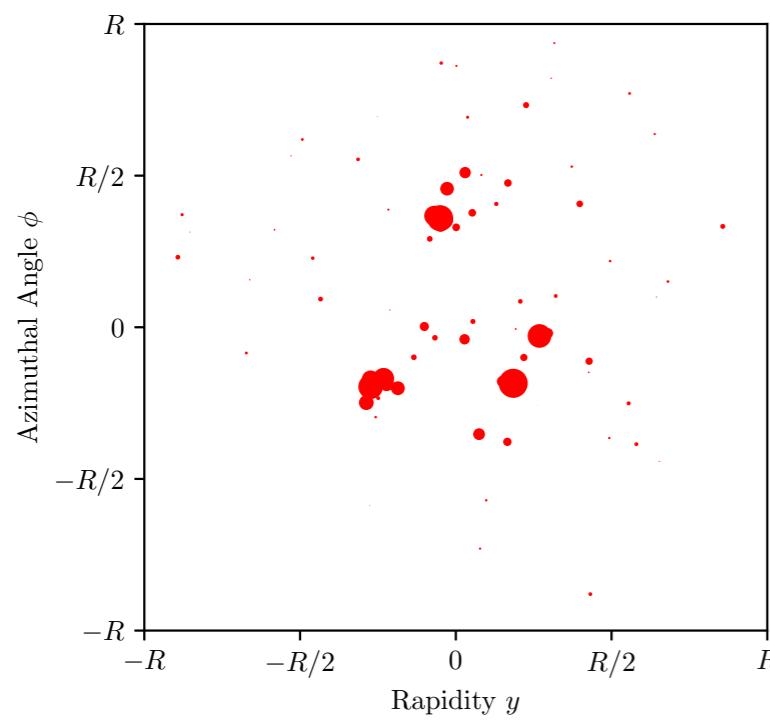
[h/t Niles-Weed, [ML4Jets 2020](#); Monge, 1781; Kantorovich, 1939; Vaserštejn, 1969; [Wikipedia](#)]

# Similarity of Two Energy Flows

$$\mathcal{E}(\hat{n}) = \sum_i \textcolor{teal}{E}_i \delta(\hat{n} - \hat{n}_i)$$

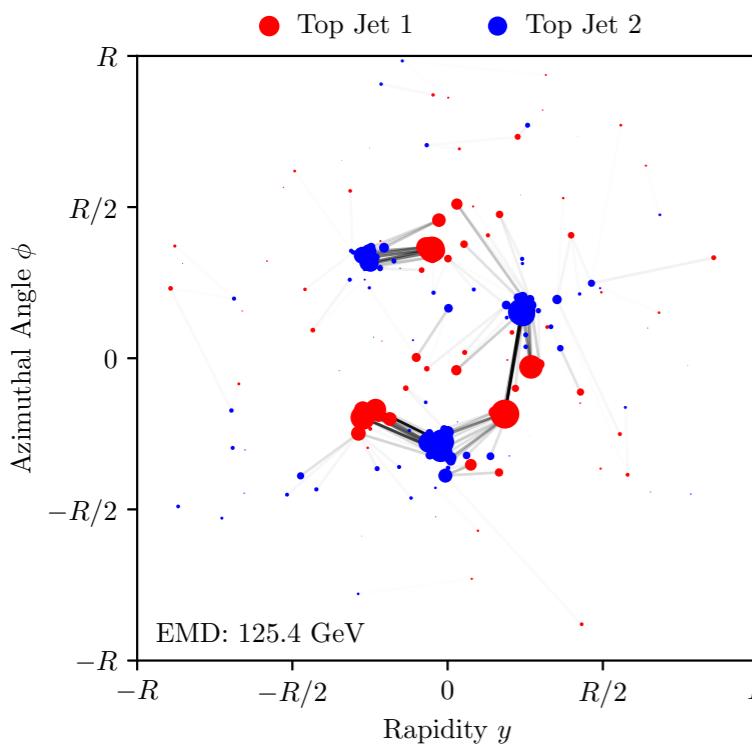
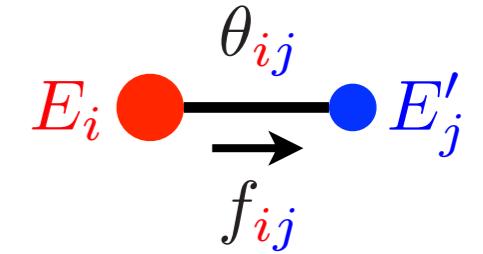


Optimal Transport:  
*Earth Mover's Distance*  
a.k.a.  $l$ -Wasserstein metric



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

# The Energy Mover's Distance



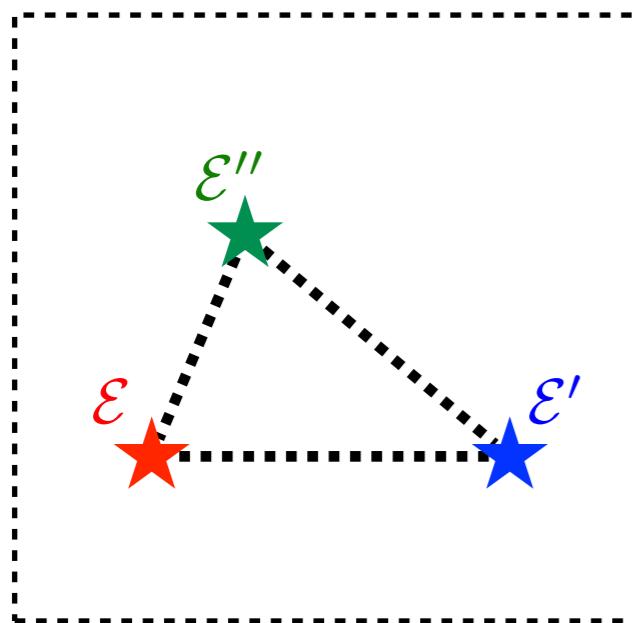
Optimal transport between energy flows...

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

↑  
in GeV

Cost to move energy

Cost to create energy



...defines a metric on the space of events

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

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

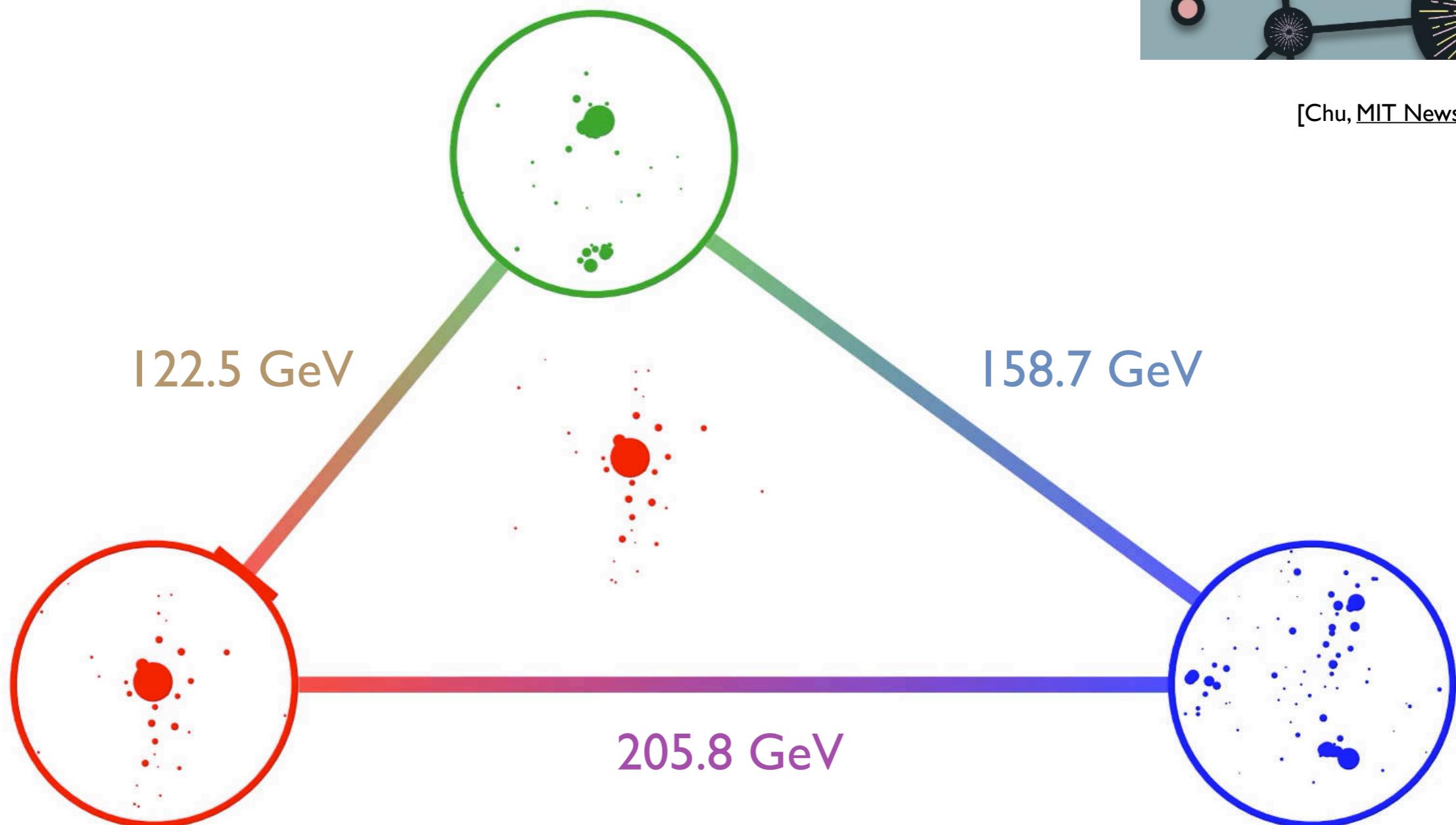
[Komiske, Metodiev, JDT, [PRL 2019](#);  
 see also Pele, Werman, [ECCV 2008](#); Pele, Taskar, [GSI 2013](#);  
 [see flavored variant in Crispim Romão, Castro, Milhano, Pedro, Vale, [EPJC 2021](#)]  
 [see computational speed up in Cai, Cheng, Craig, Craig, [PRD 2020](#)]



# Similarity of Three Energy Flows



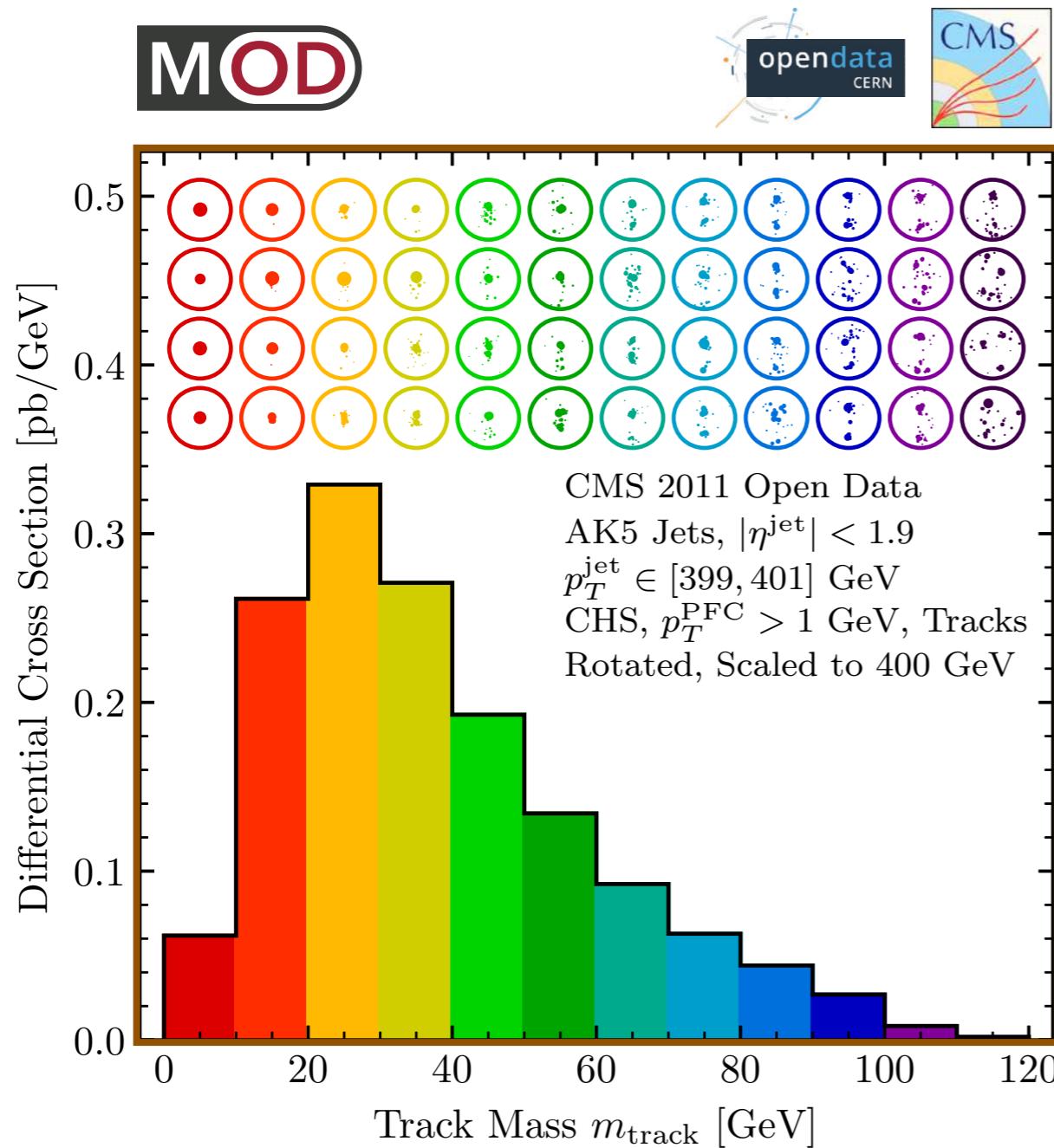
[Chu, MIT News July 2019]



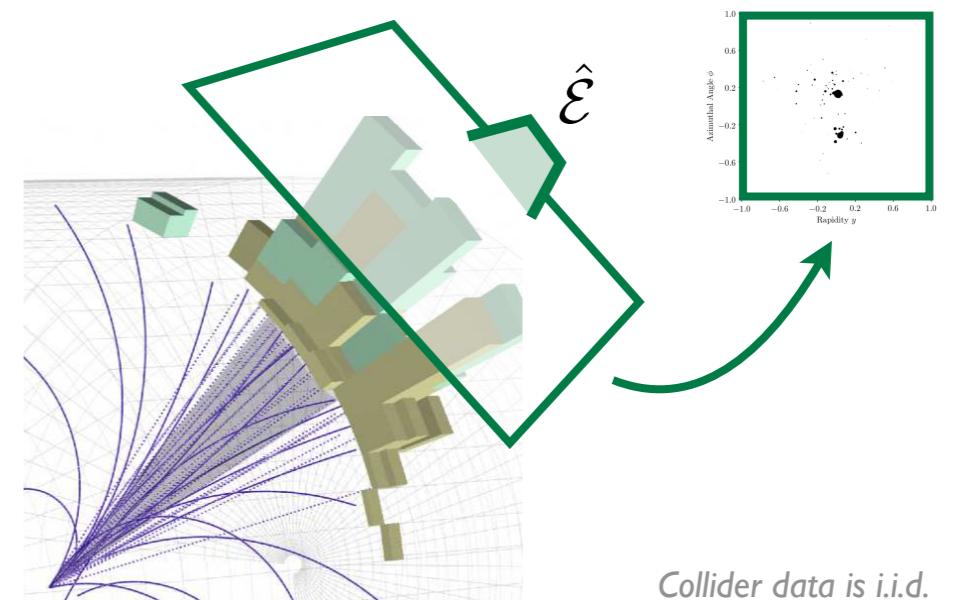
[Komiske, Metodiev, JDT, [PRL 2019](#); code at Komiske, Metodiev, JDT, [energyflow.network](#); see alternative graph network approach in Mullin, Pacey, Parker, White, Williams, [JHEP 2021](#)]



# The Forest and the Trees



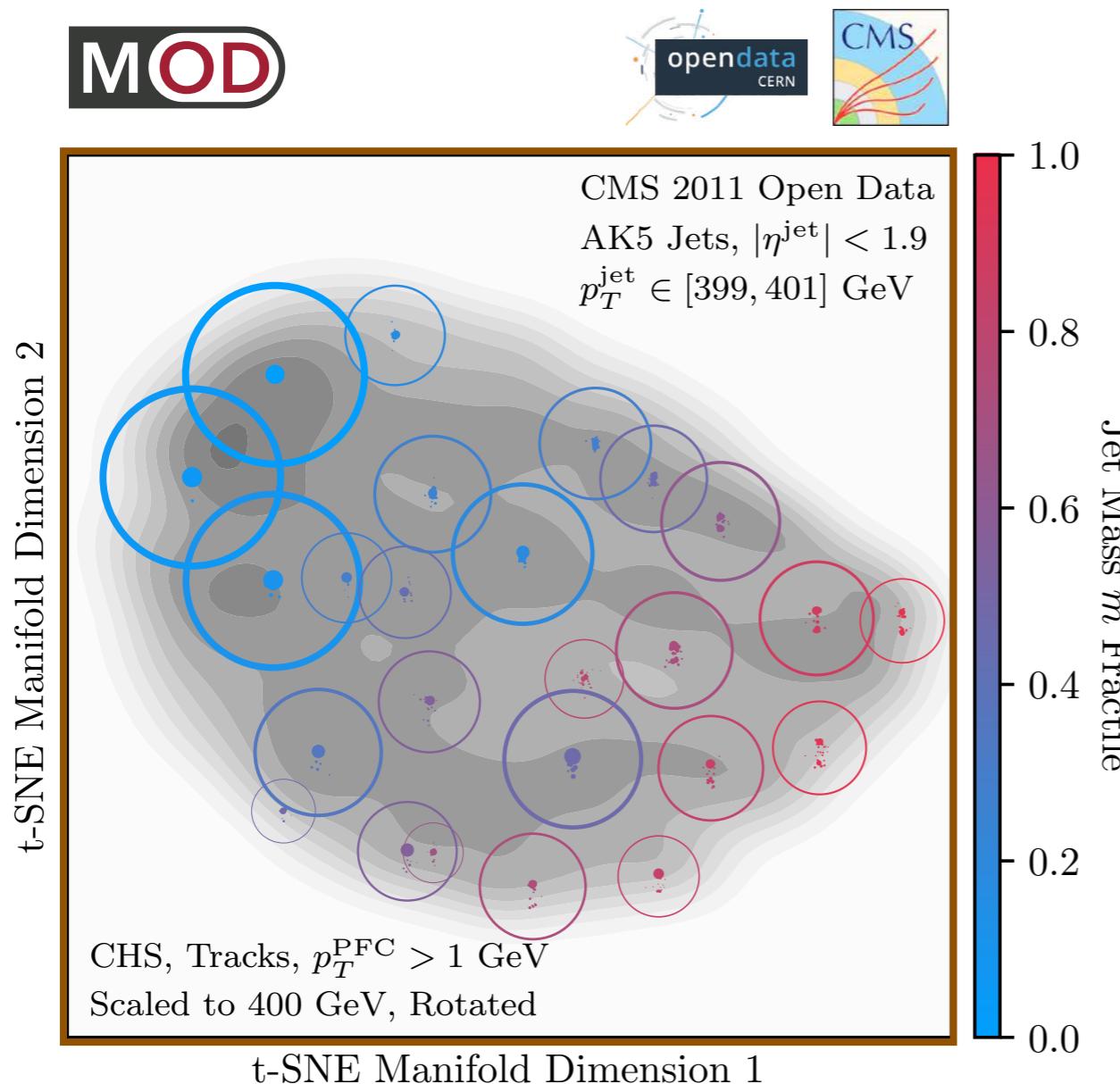
A *Histogram of Observables*



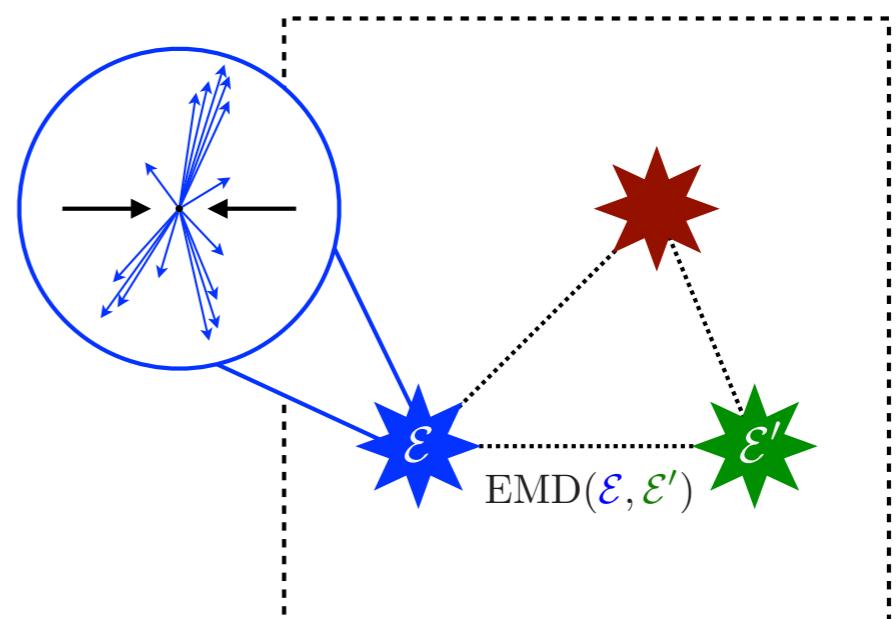
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;  
using CMS Open Data]



# Building the Forest from the Trees



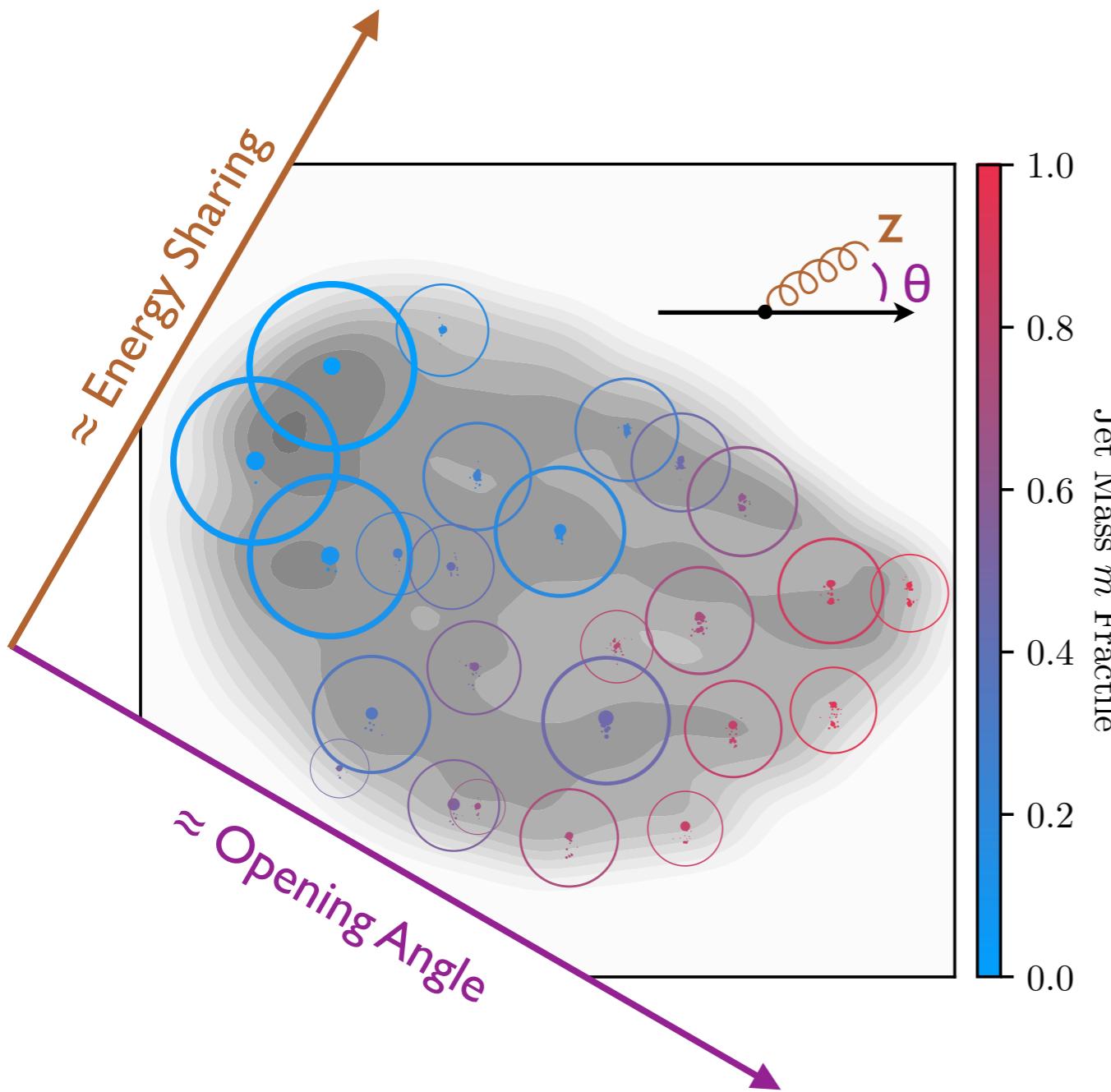
*The Space of Energy Flows*



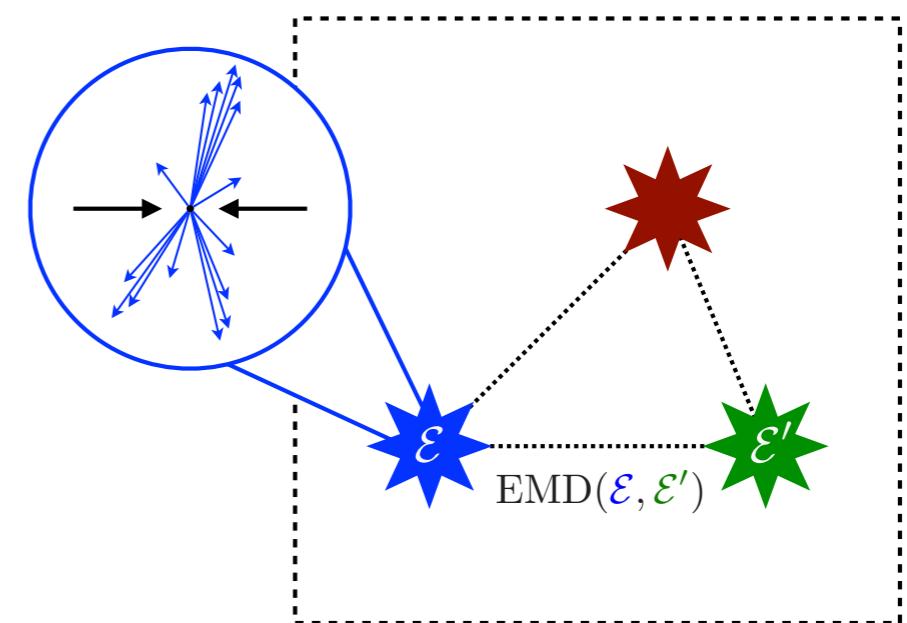
[Komiske, Mastandrea, Metodiev, Naik, JDT, [PRD 2020](#);  
using van der Maaten, Hinton, [JMLR 2008](#); using [CMS Open Data](#)]



# Building the Forest from the Trees



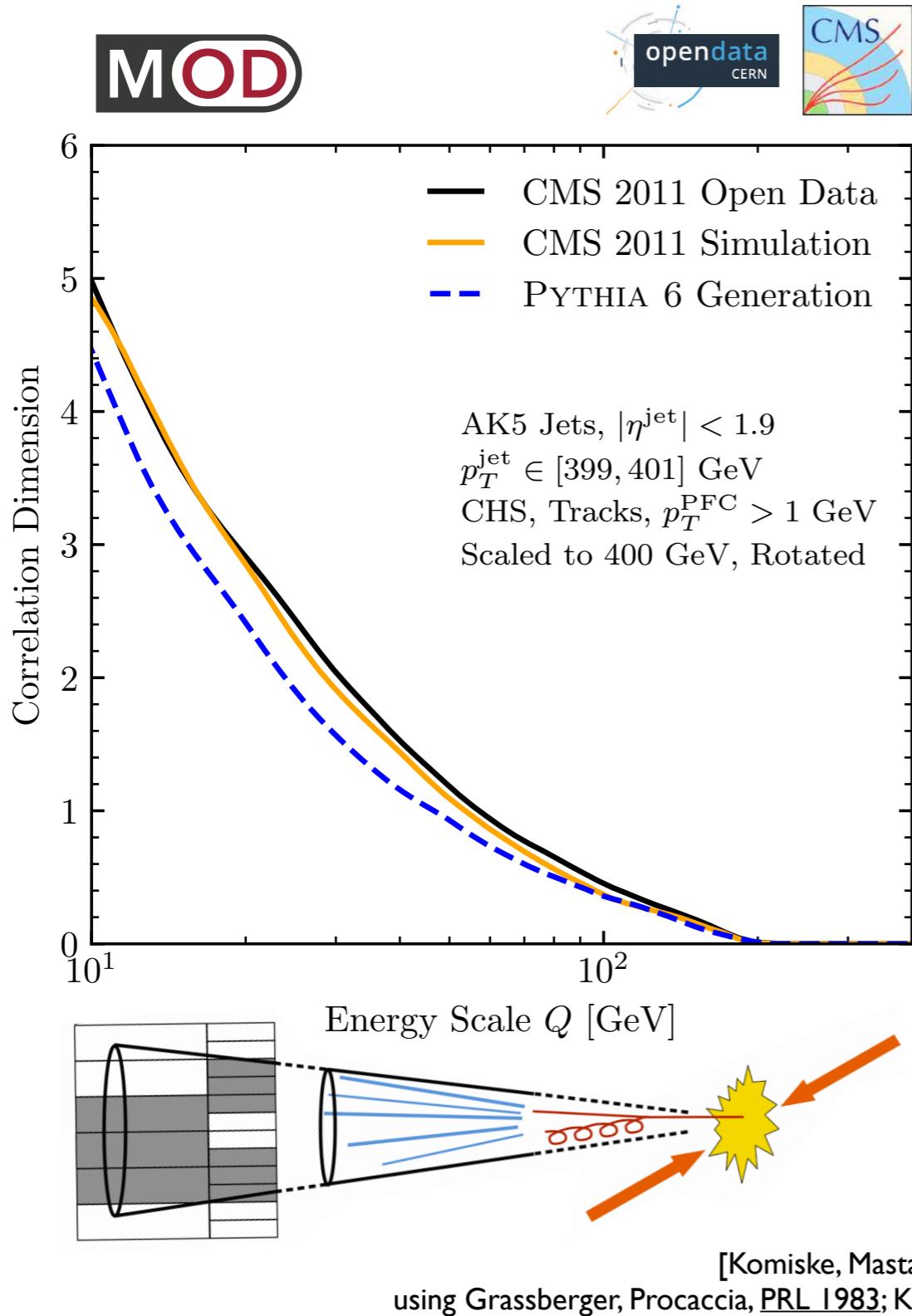
*The Space of Energy Flows*



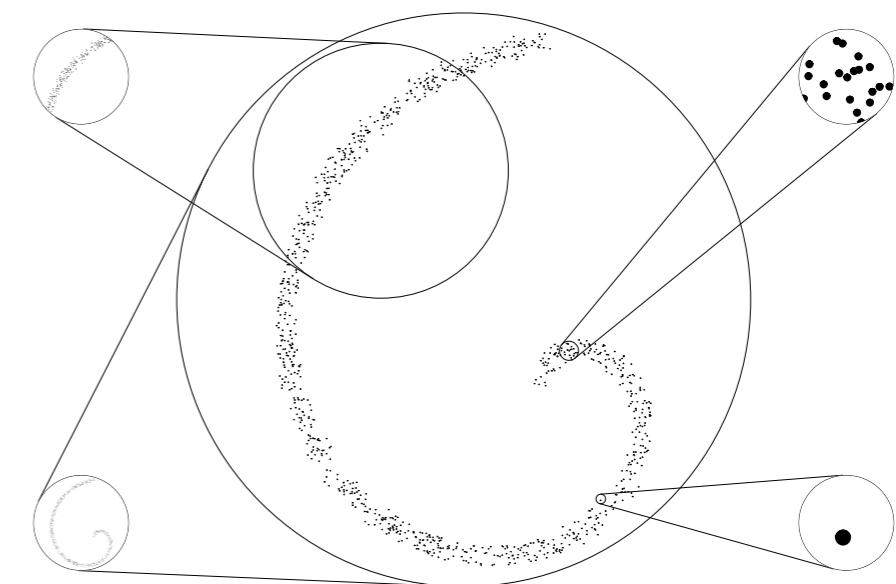
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;  
using van der Maaten, Hinton, JMLR 2008; using CMS Open Data]

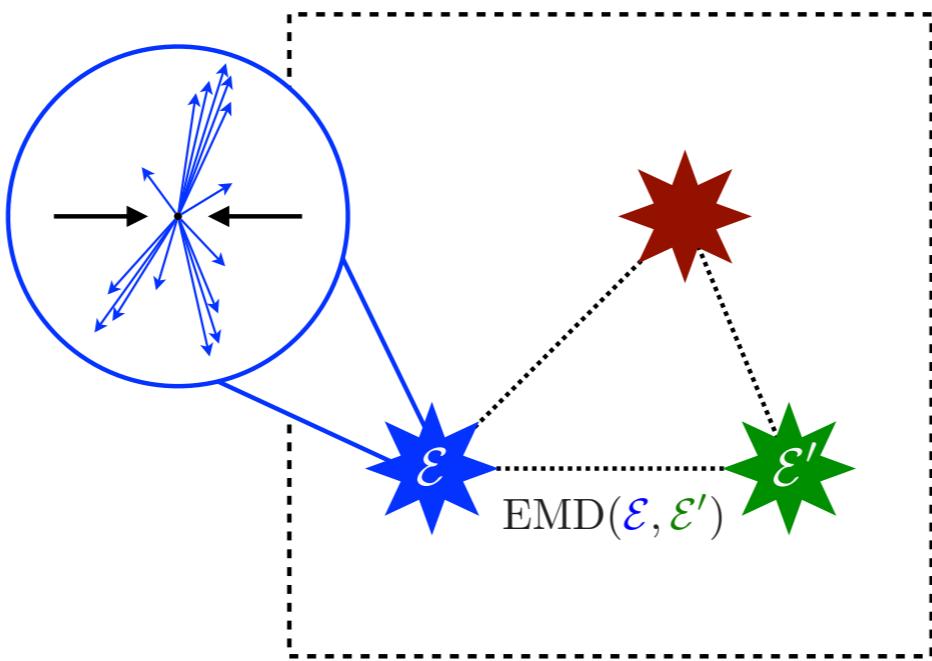


# A Super-Fractal Forest made from Trees

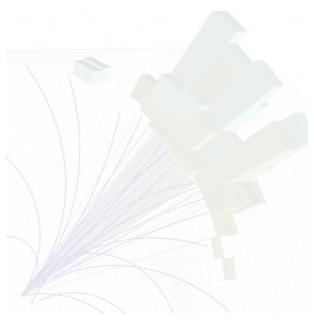


*Dimension of Space of Energy Flows*

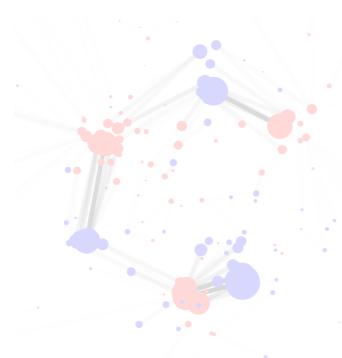




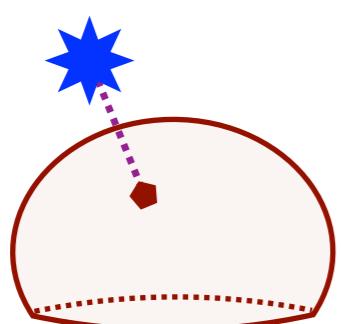
*Viewed through the data science lens,  
the EMD unlocks a suite of  
geometric analysis strategies*



## Going with the (Energy) Flow



## The Energy Mover's Distance

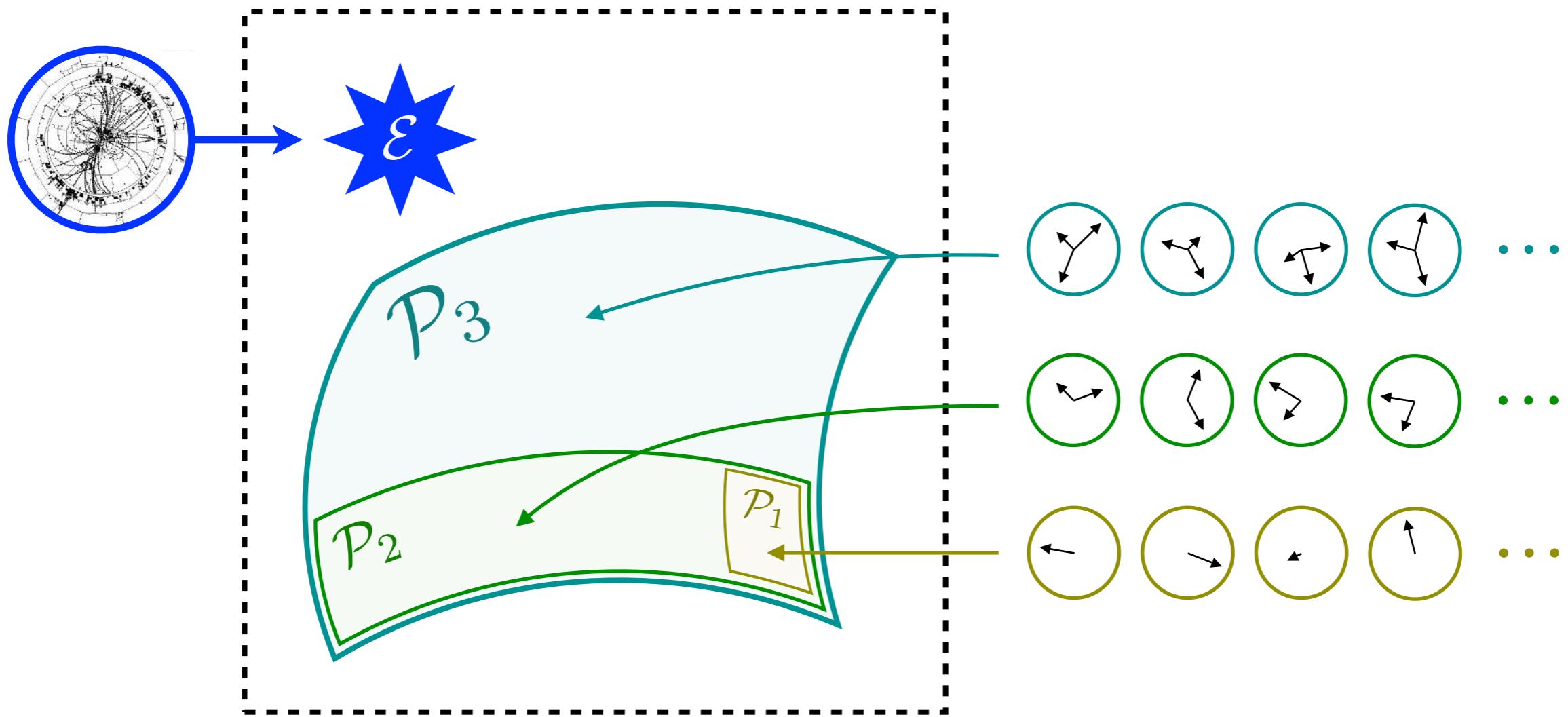


## Revealing a Hidden Geometry

*Given a metric space, the first geometric object  
you might think to construct is...*

# Introducing N-particle Manifolds

$\mathcal{P}_N$  = set of all N-particle configurations

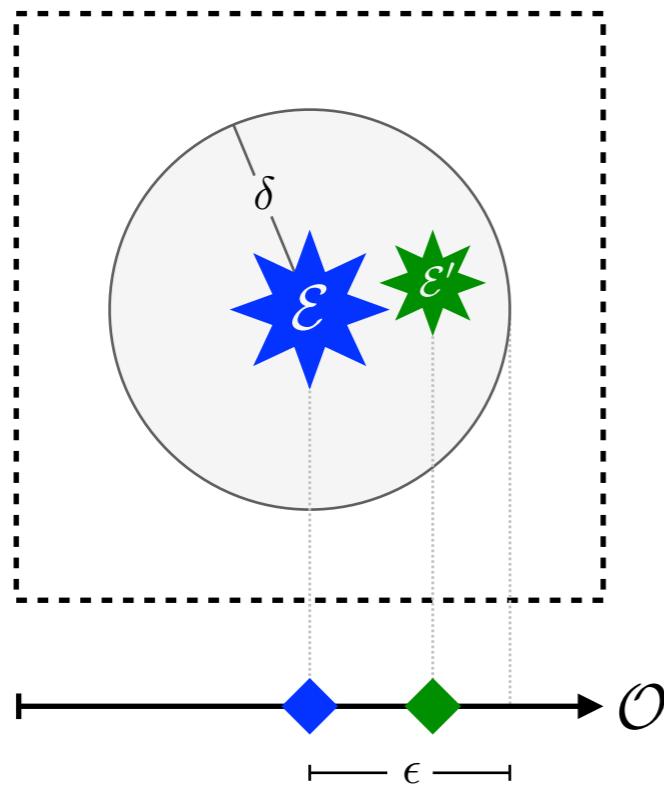


$\mathcal{P}_N \supset \mathcal{P}_{N-1} \supset \dots \supset \mathcal{P}_2 \supset \mathcal{P}_1$  by soft/collinear limits

[see related discussion in Larkoski, Melia, [PRD 2020](#)]

# Introducing N-particle Manifolds

$\mathcal{P}_N$  = set of all N-particle configurations



## Infrared & Collinear Safety

≈ calculable in perturbative quantum field theory

*iS\**

## Continuity in EMD Space

[Komiske, Metodiev, JDT, JHEP 2020]

[Sterman, Weinberg, PRL 1977; Sterman, PRD 1979]

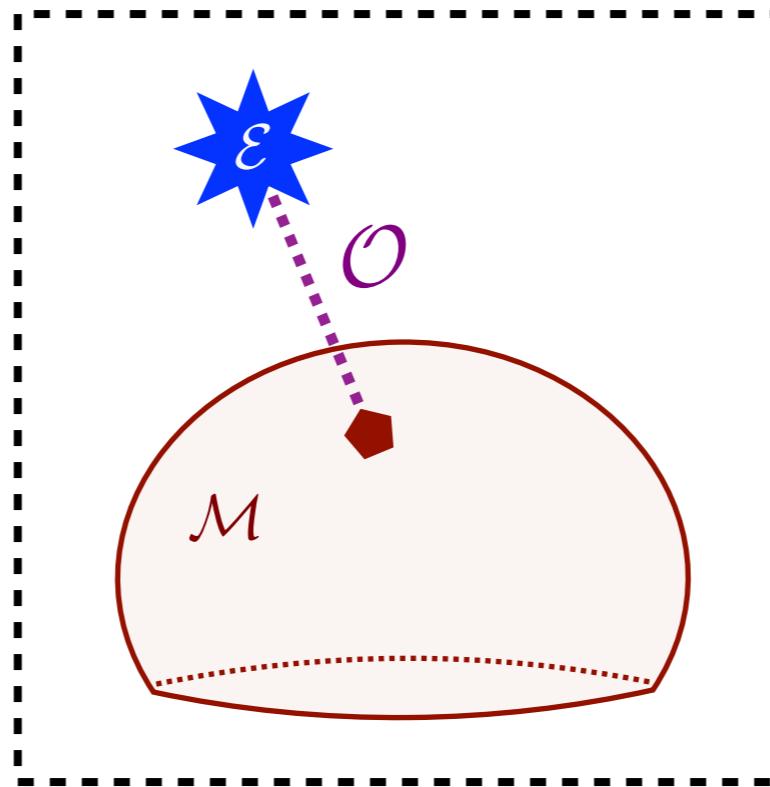
[see also Banfi, Salam, Zanderighi, JHEP 2005; Larkoski, Marzani, JDT, PRD 2015]

$\mathcal{P}_N \supset \mathcal{P}_{N-1} \supset \dots \supset \mathcal{P}_2 \supset \mathcal{P}_1$  by soft/collinear limits

[see related discussion in Larkoski, Melia, PRD 2020]

# Manifolds for Observables

One Event



Set of Events

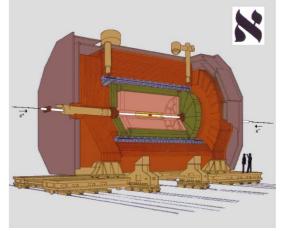
Distance of Closest Approach  $\Rightarrow$  Observable

$$O(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{M}} \text{EMD}(\mathcal{E}, \mathcal{E}')$$

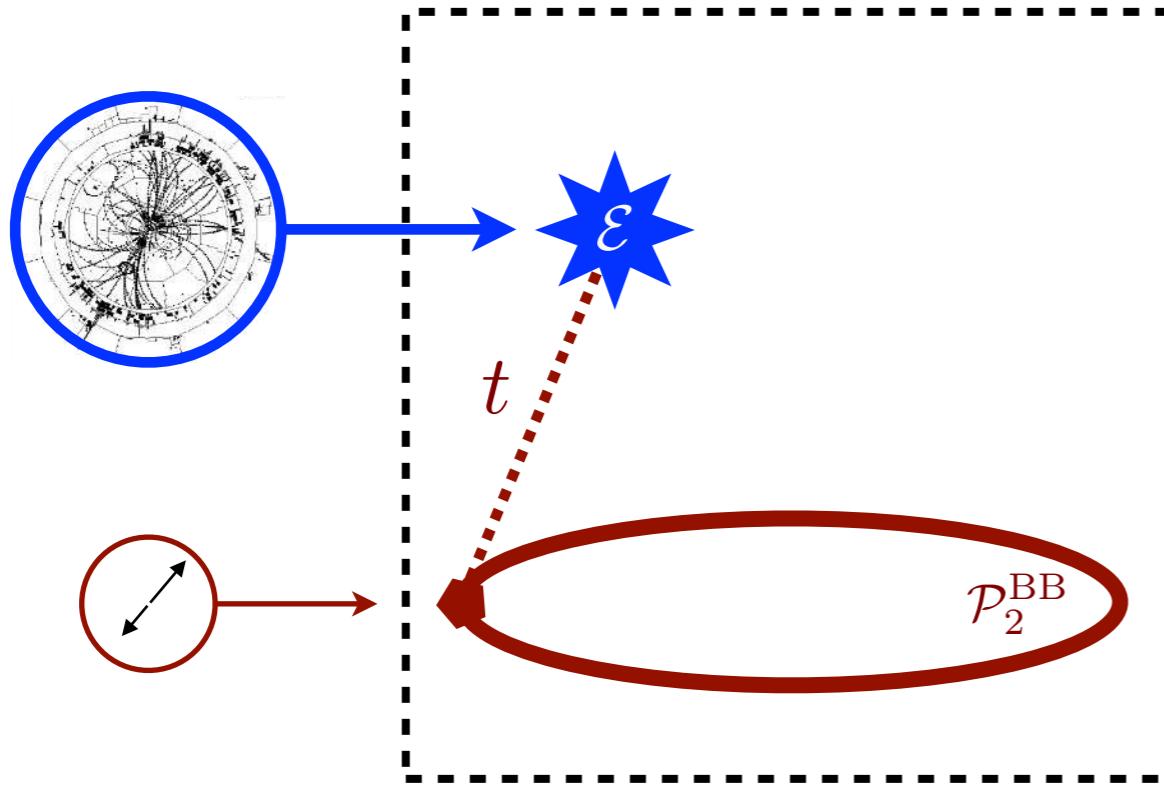
[Komiske, Metodiev, JDT, [JHEP 2020](#)]

# E.g. Thrust

How dijet-like is an event?



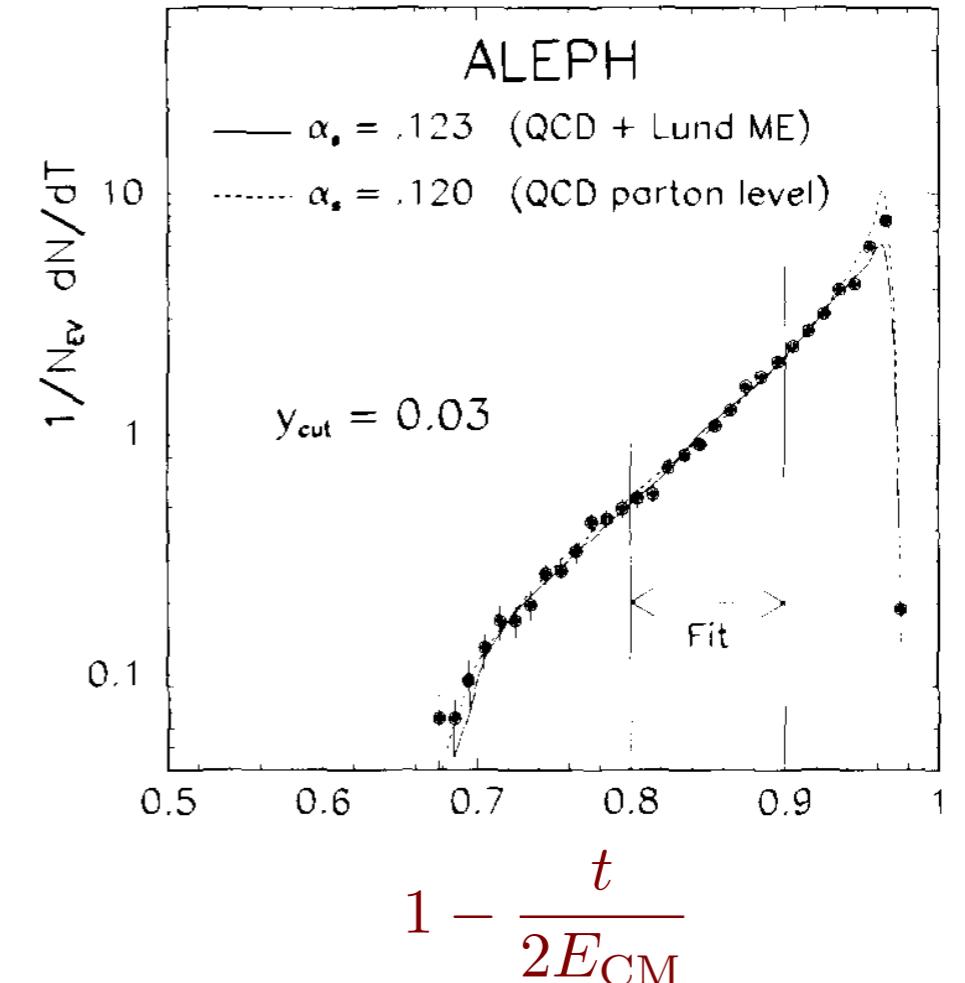
$$t(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{P}_2^{\text{BB}}} \text{EMD}_2(\mathcal{E}, \mathcal{E}')$$



All Back-to-Back Two Particle Configurations

$$\mathcal{P}_2^{\text{BB}} = \left\{ \begin{array}{c} \text{Diagram 1} \\ \text{Diagram 2} \\ \text{Diagram 3} \\ \text{Diagram 4} \\ \dots \end{array} \right\}$$

(using  $\beta=2$  EMD variant)



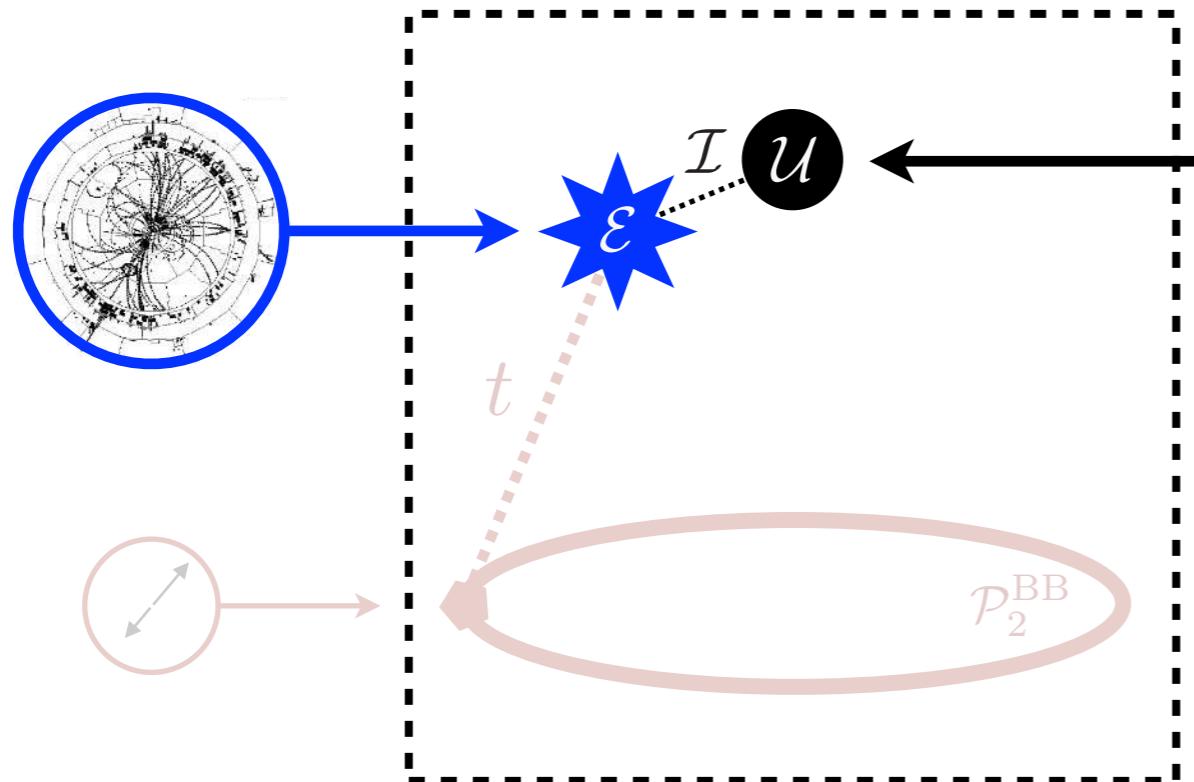
$$1 - \frac{t}{2E_{\text{CM}}}$$

$$\text{cf. } T(\mathcal{E}) = \max_{\hat{n}} \frac{\sum_i |\vec{p}_i \cdot \hat{n}|}{\sum_j |\vec{p}_j|}$$

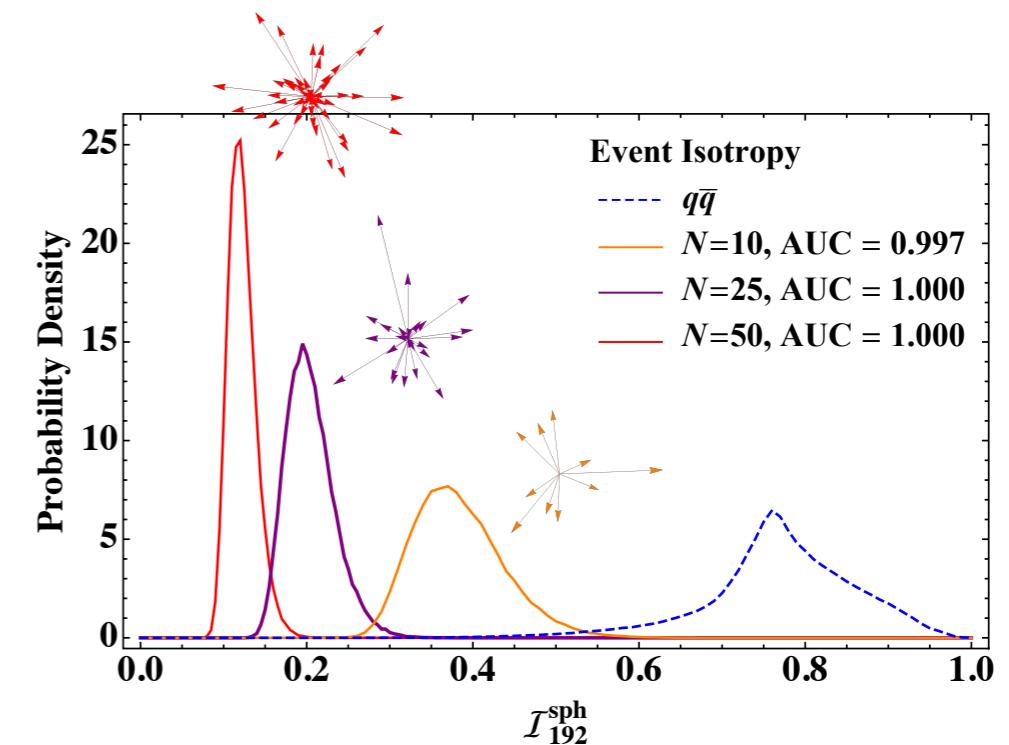
[Komiske, Metodiev, JDT, JHEP 2020]  
 [Brandt, Peyrou, Sosnowski, Wroblewski, PL 1964; Farhi, PRL 1977; ALEPH, PLB 1991]

# New! Event Isotropy

How isotropic is an event?



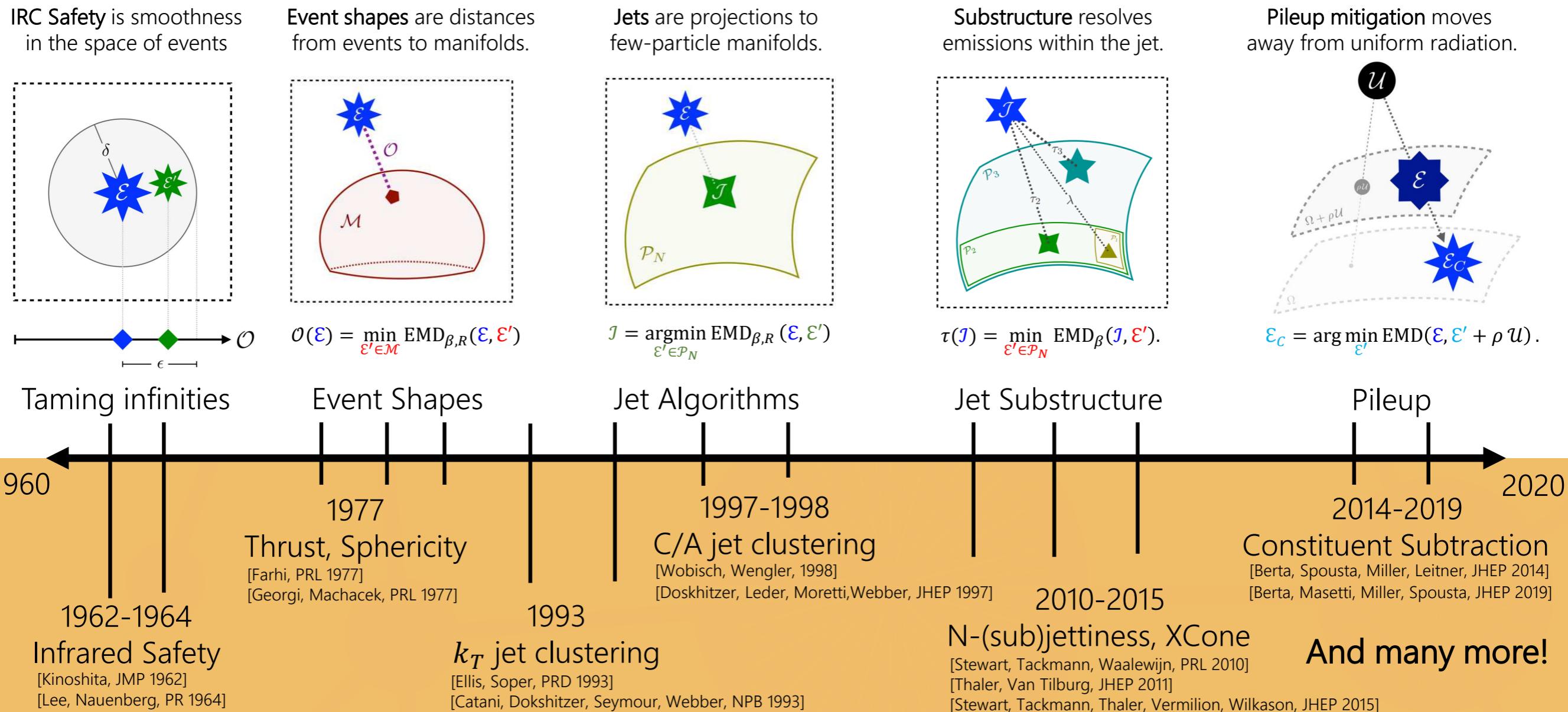
$$\mathcal{I}(\mathcal{E}) = \text{EMD}(\mathcal{E}, \mathcal{U})$$



[Cesarotti, JDT, [JHEP 2020](#);  
see also Cesarotti, Reece, Strassler, [JHEP 2021](#)]



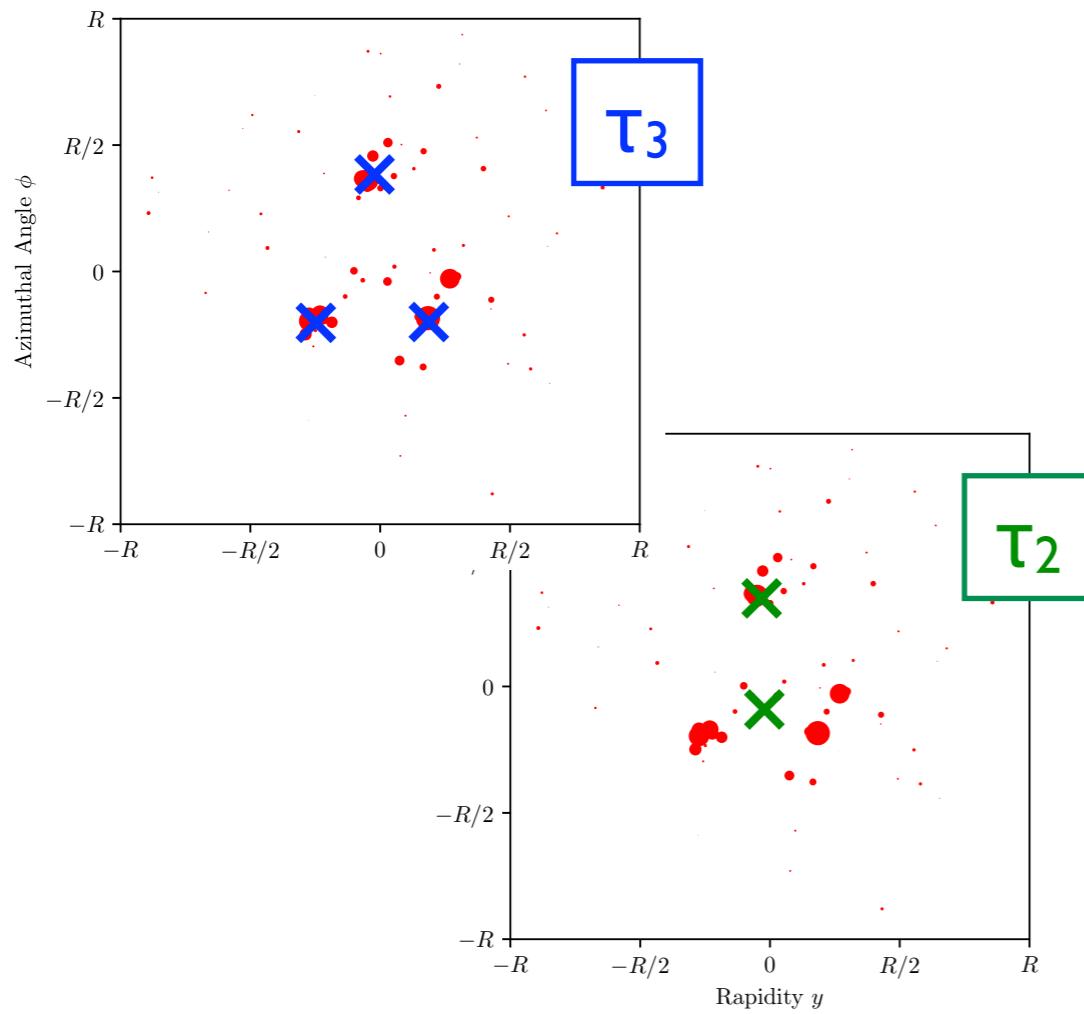
# Six Decades of Collider Physics Translated into a New Geometric Language!



# N-subjettiness

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

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



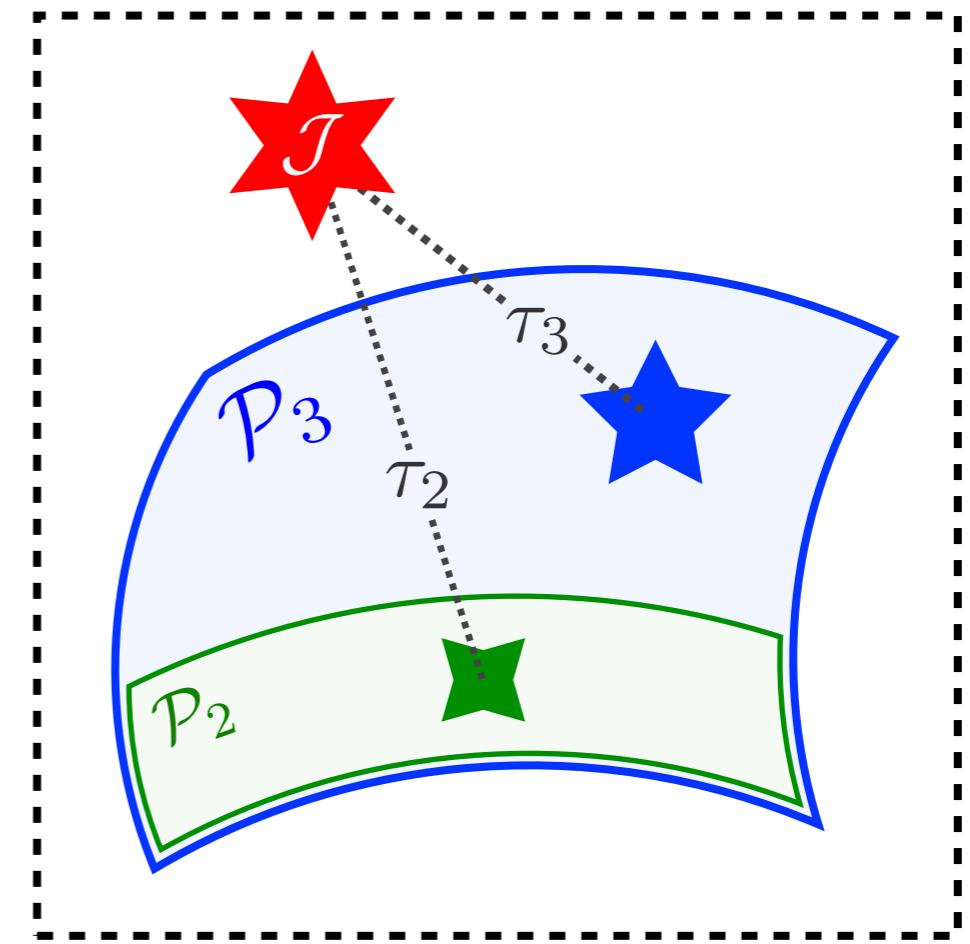
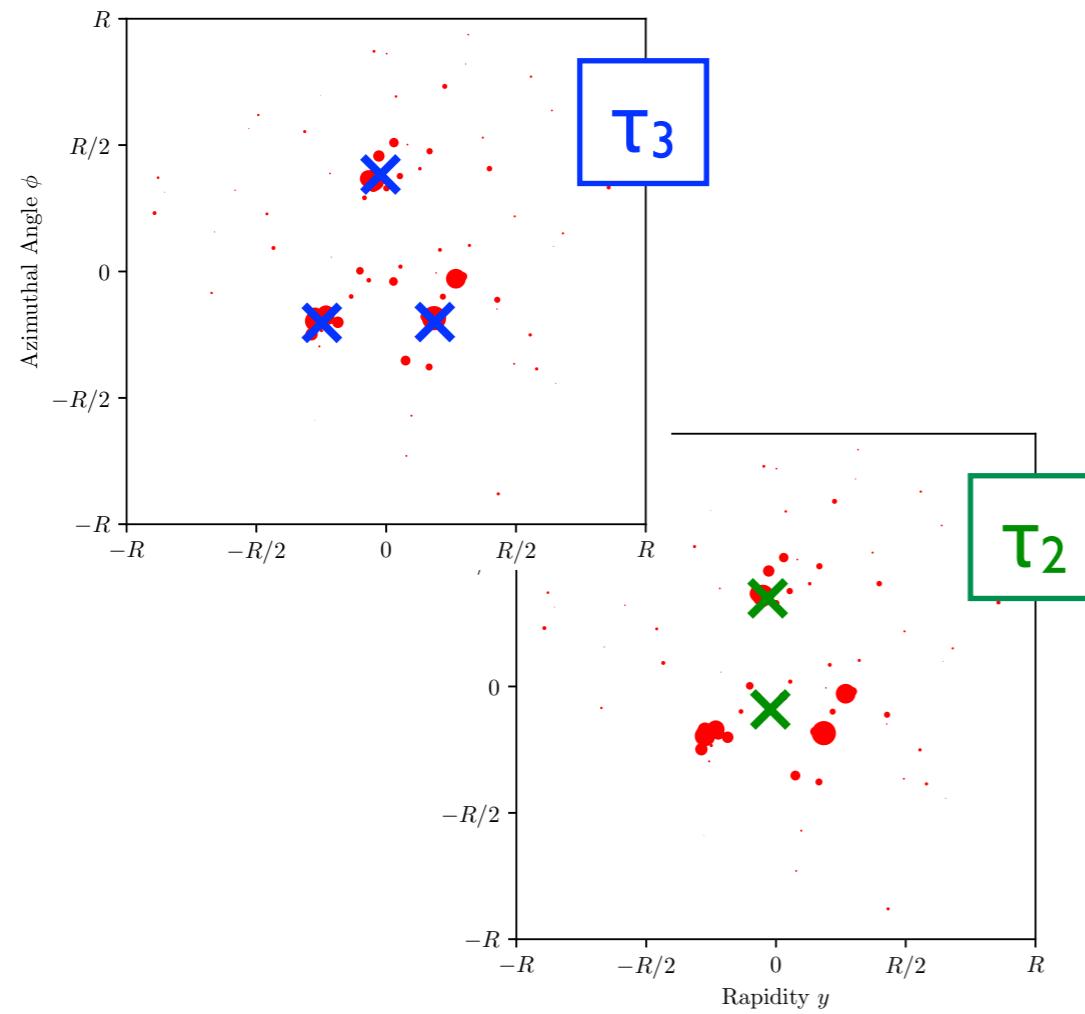
[JDT, Van Tilburg, [JHEP 2011](#), [JHEP 2012](#);  
based on Brandt, Dahmen, [ZPC 1979](#); Stewart, Tackmann, Waalewijn, [PRL 2010](#)]



# N-subjettiness = Point to Manifold EMD

*...is secretly an optimal transport problem*

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



[JDT, Van Tilburg, [JHEP 2011](#), [JHEP 2012](#);  
rephrased in the language of Komiske, Metodiev, JDT, [PRL 2019](#)]

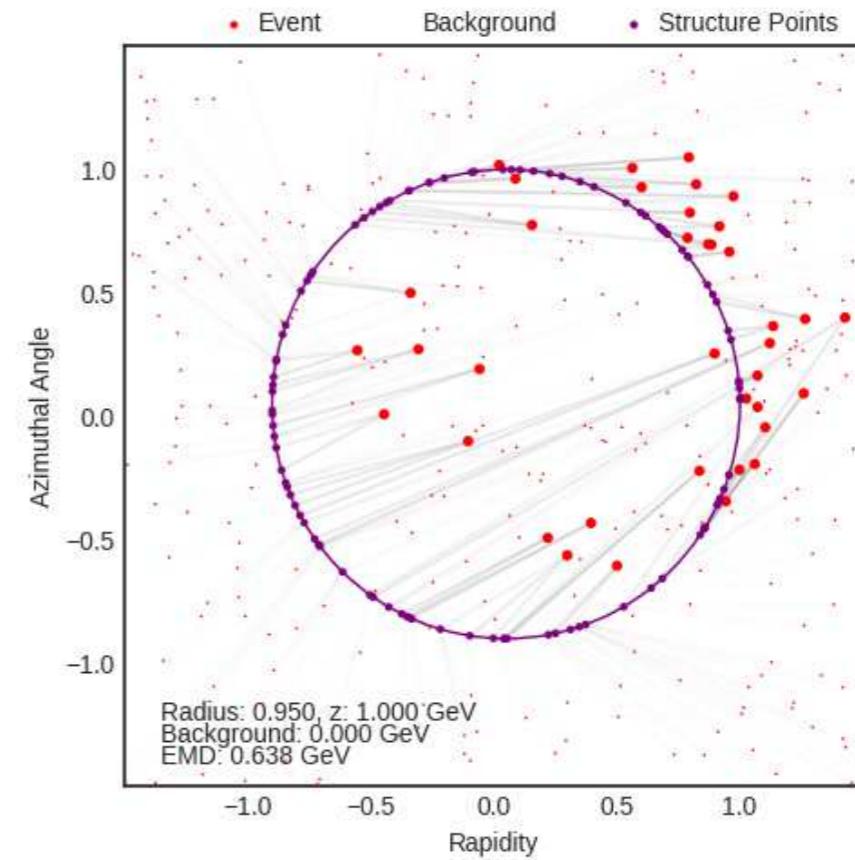
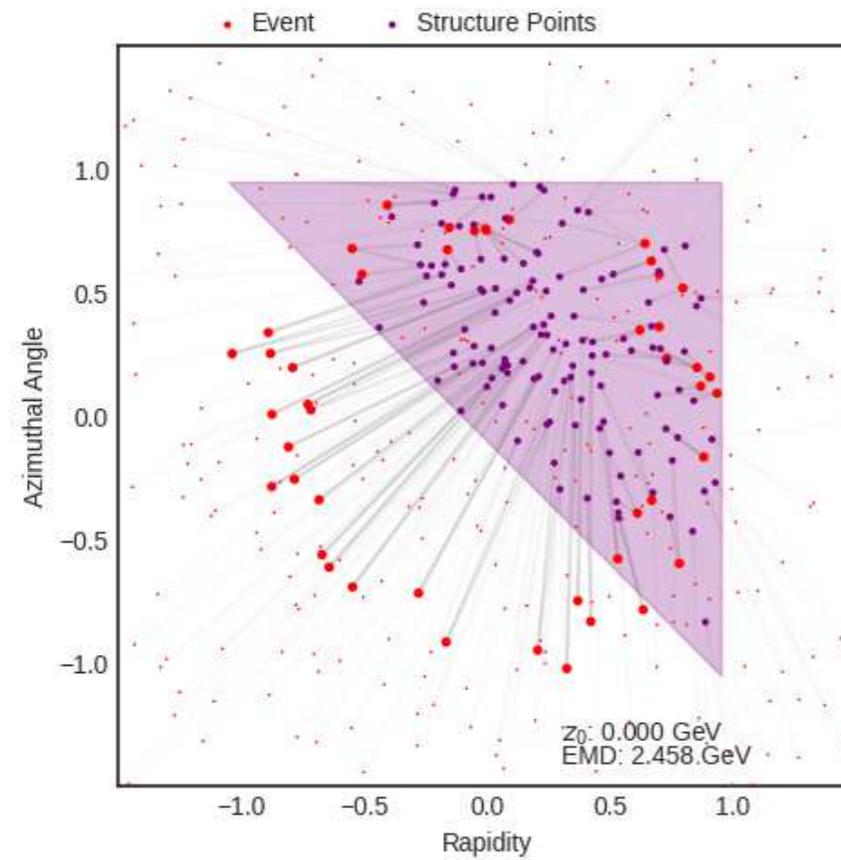


# Deep Manifold Learning

*Optimal transport meets gradient descent*

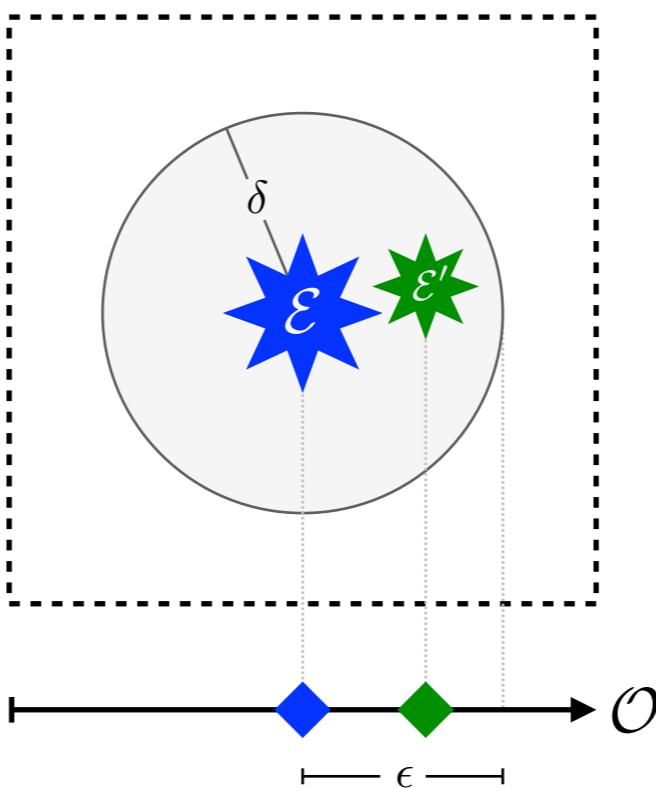
$$\mathcal{O}(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{M}} \text{EMD}(\mathcal{E}, \mathcal{E}')$$

*How triangle-like / ring-like is this jet?*



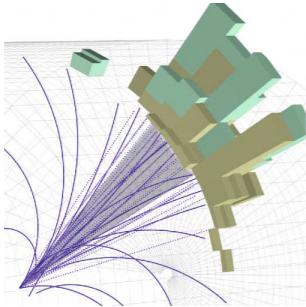
[Ba, Dogra, Gambhir, JDT, in progress;  
inspired by Tankala, Tasissa, Murphy, Ba, [arXiv 2020](#)]





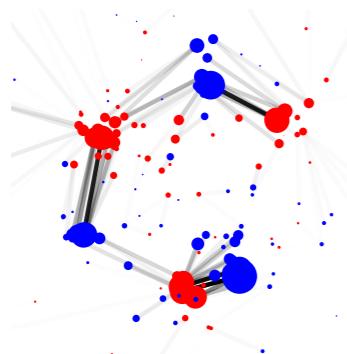
We are just beginning to leverage the  
*conceptual richness* of optimal transport  
for high-energy physics application

# Summary



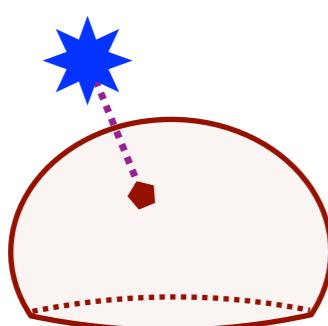
## Going with the (Energy) Flow

*Restricting our attention to  $IRC$  safe information  
is a theoretically motivated data analysis strategy*



## The Energy Mover's Distance

*Optimal transport allows us to triangulate the space  
of collider events and define an emergent geometry*

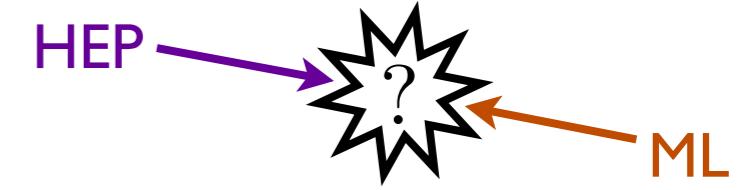


## Revealing a Hidden Geometry

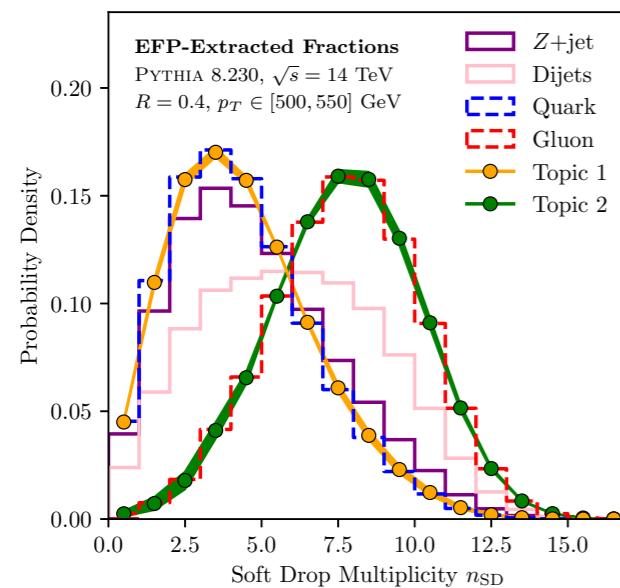
*We can gain new perspectives on concepts/techniques  
in  $QFT$  and collider physics from the last half century*

# *Backup Slides*

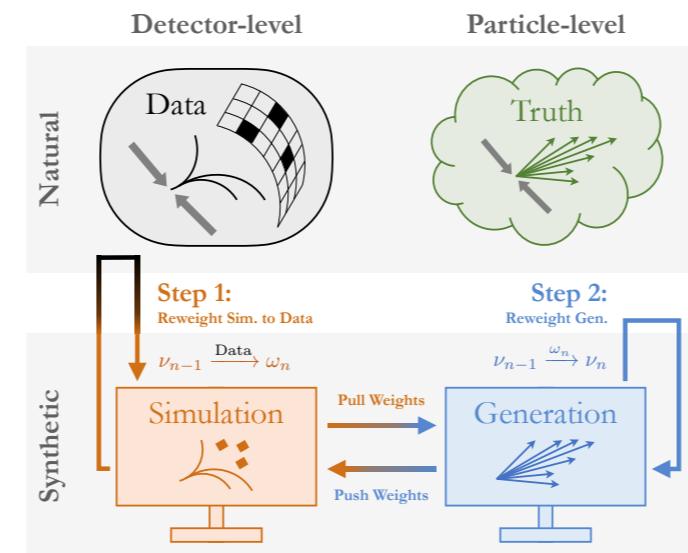
# Recent Collisions



## Quark/Gluon Definitions via Blind Source Separation



## Detector Deconvolution via Binary Classification

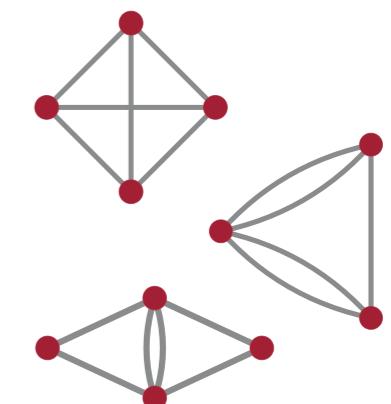


[Komiske, Metodiev, JDT, [JHEP 2018](#);  
Brewer, JDT, Turner; [PRD 2021](#)]

[Andreassen, Komiske, Metodiev,  
Nachman, JDT, [PRL 2020](#)]

## Kinematic Decomposition via Graph Theory

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



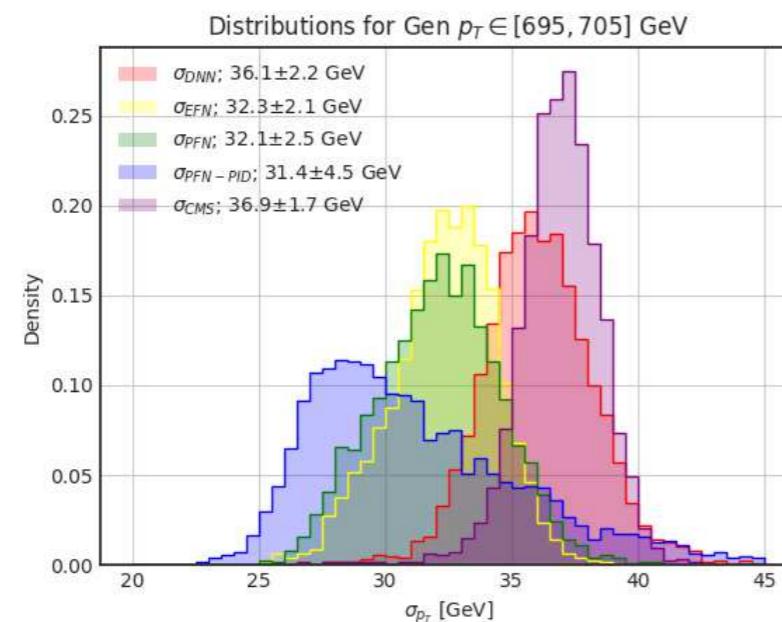
[Komiske, Metodiev, JDT,  
[JHEP 2018, PRD 2020](#)]

*High Energy Physics  $\leftrightarrow$  Mathematics, Statistics & Computer Science*

# Ongoing Collisions

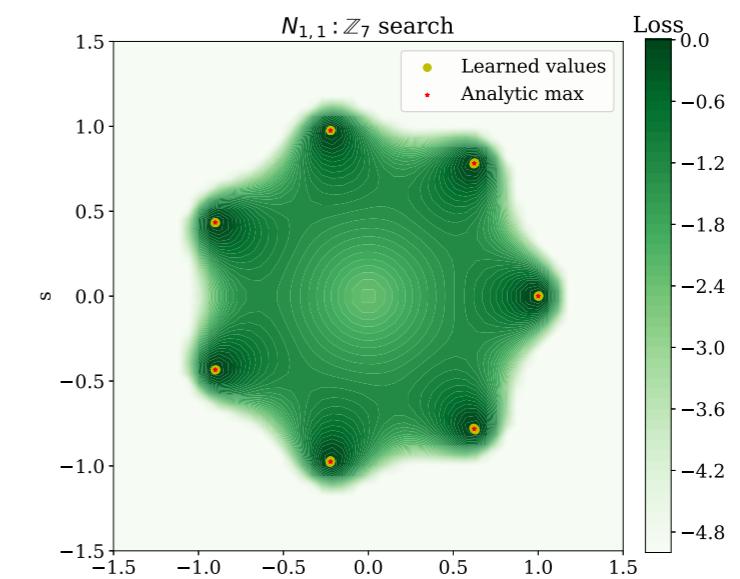


## Frequentist Jet Calibration via Gaussian Ansatz



[Nachman, Gambhir, JDT, in progress]

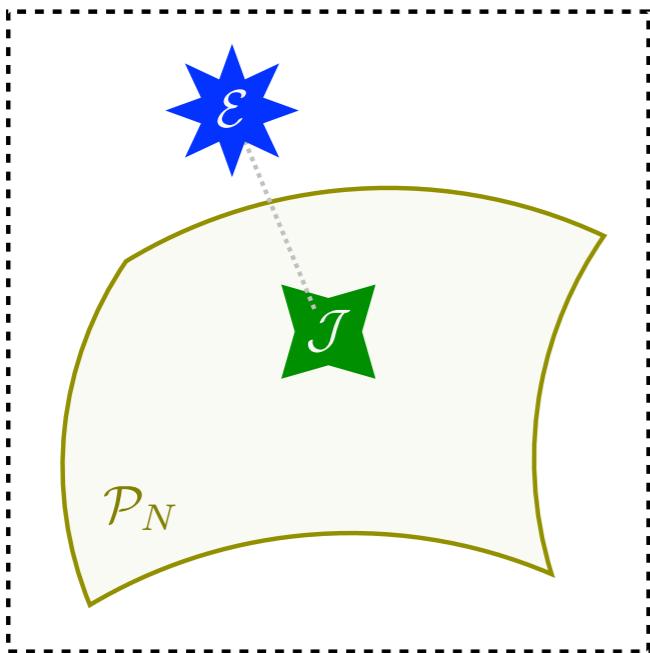
## Symmetry Discovery via Adversarial Learning



[Desai, Nachman, JDT, NeurIPS 2021 ML4PS]

*High Energy Physics  $\leftrightarrow$  Mathematics, Statistics & Computer Science*

# More Fun with N-particle Manifolds



## N-jettiness

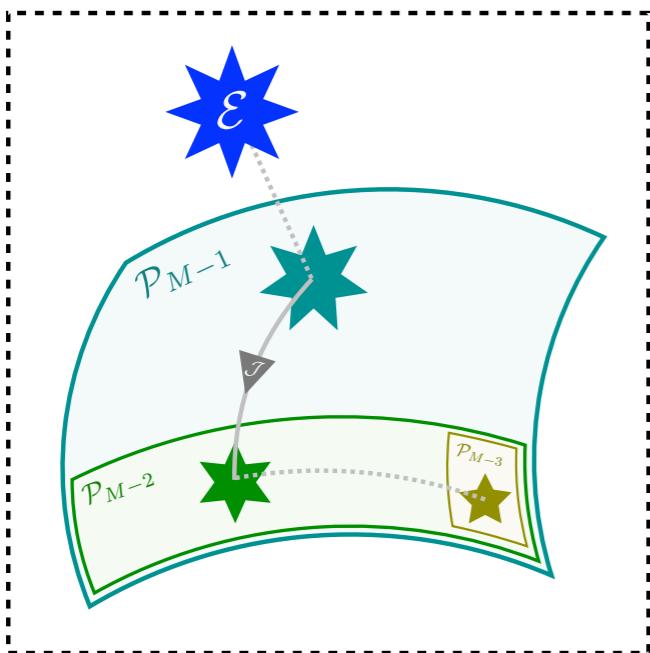
*Distance of closest approach to N-particle manifold*

[Brandt, Dahmen, [ZPC 1979](#); Stewart, Tackmann, Waalewijn, [PRL 2010](#)]

## Exclusive Cone Jet Finding

*Point of closest approach on N-particle manifold*

[Stewart, Tackmann, JDT, Vermilion, Wilkason, [JHEP 2015](#)]



## Sequential Jet Recombination

*Iteratively stepping between various N-particle manifolds*

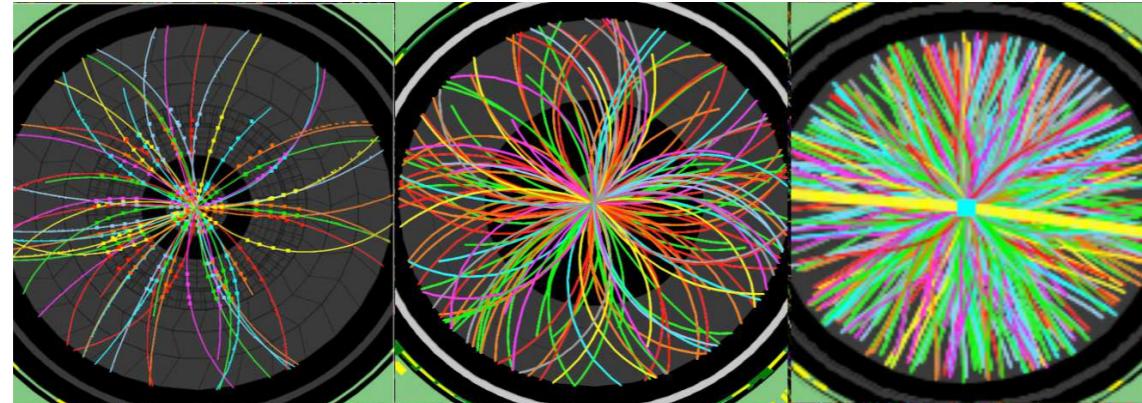
[Catani, Dokshitzer, Seymour, Webber, [NPB 1993](#); Ellis, Soper, [PRD 1993](#)]

[Dokshitzer, Leder, Moretti, Webber, [JHEP 1997](#); Wobisch, Wengler, [arXiv 1999](#)]

[Butterworth, Couchman, Cox, Waugh, [CPC 2003](#); Larkoski, Neill, JDT, [JHEP 2014](#)]

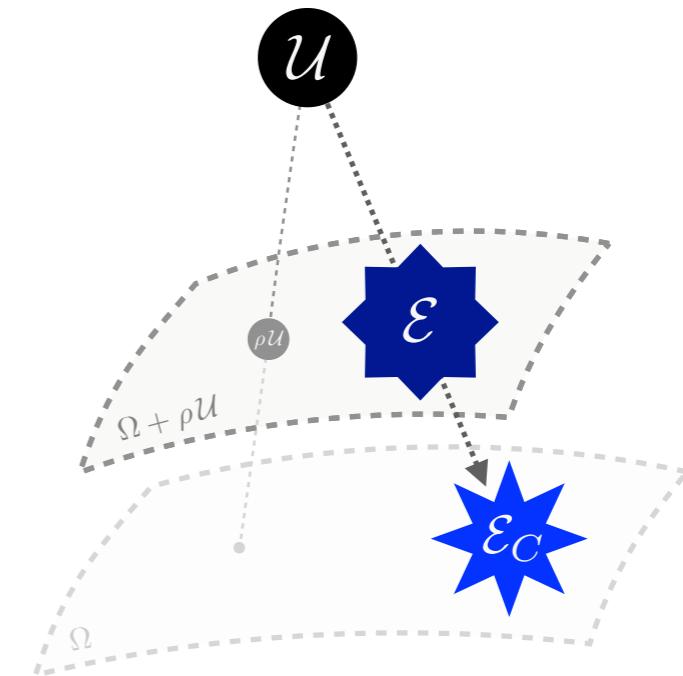
[Komiske, Metodiev, JDT, [JHEP 2020](#)]

# Pileup Mitigation



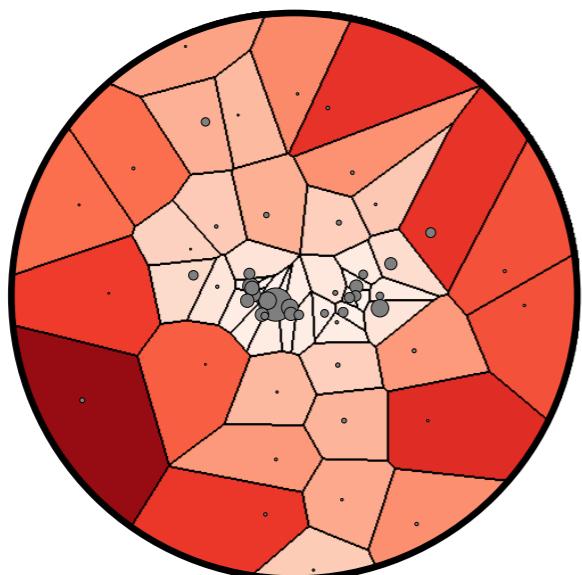
[see review in Soyez, PR 2019]

Uniform event contamination from overlapping proton-proton collisions



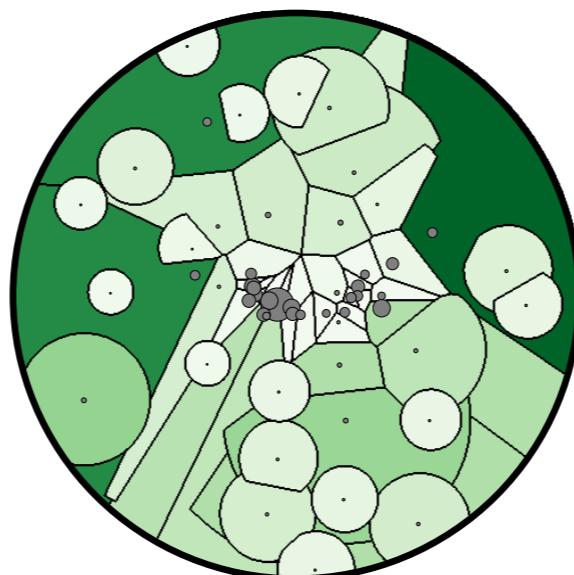
Pileup Mitigation:  
“Move away” from uniform event

Voronoi



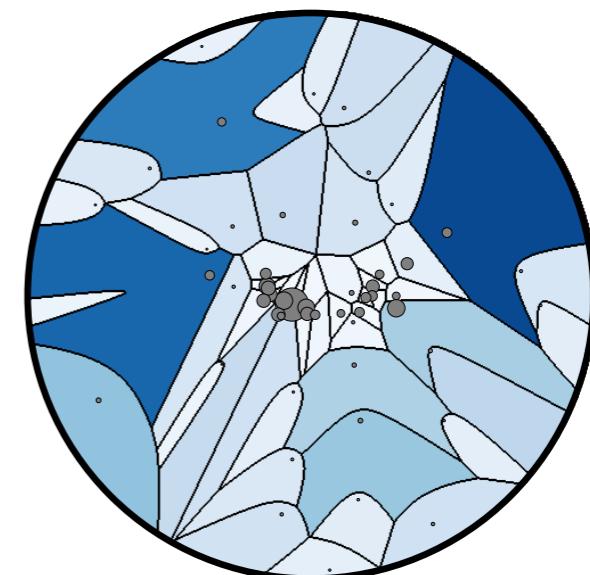
[Cacciari, Salam, Soyez, JHEP 2008]

Constituent Subtraction



[Berta, Spousta, Miller, Leitner, JHEP 2014]

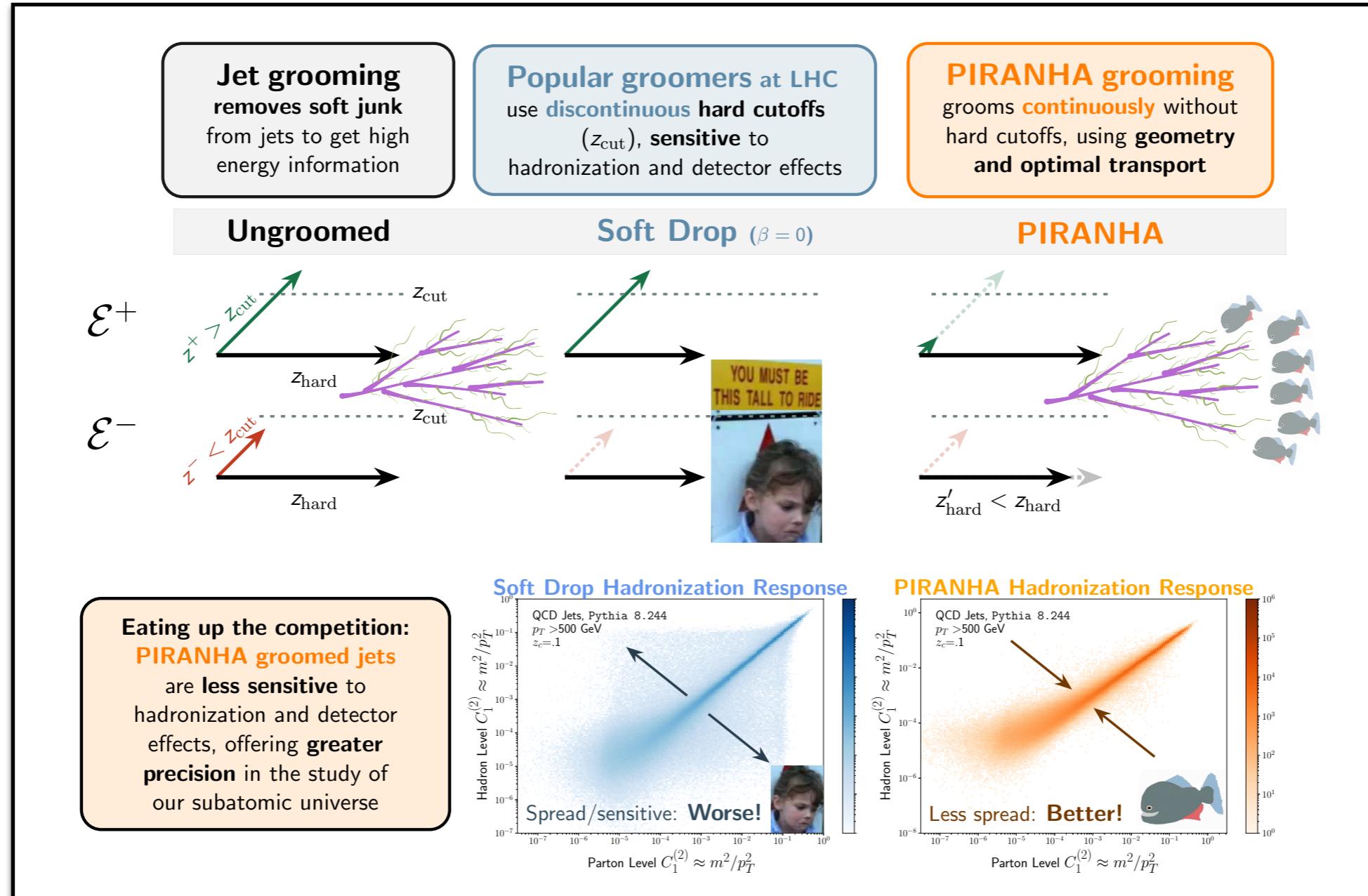
Apollonius



[Komiske, Metodiev, JDT, JHEP 2020]

# Pileup and Infrared Radiation AnNiHilAtion

*Recursive Safe Subtraction: tree-based approx. to optimal transport grooming*



[Slides from Sam Alipour-fard]  
[Alipour-fard, Komiske, Metodiev, JDT, in progress]

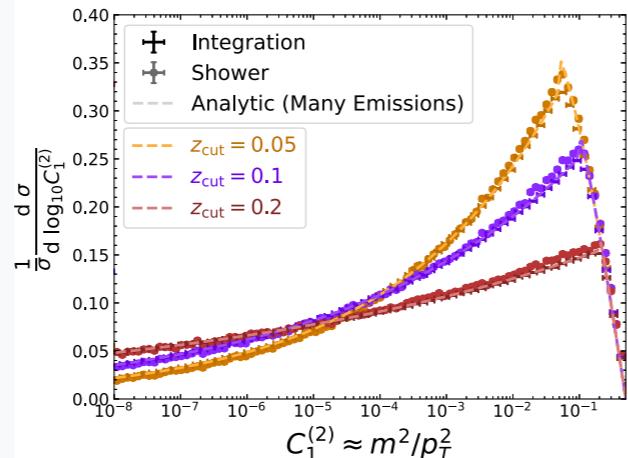


# Pileup and Infrared Radiation AnNiHilAtion

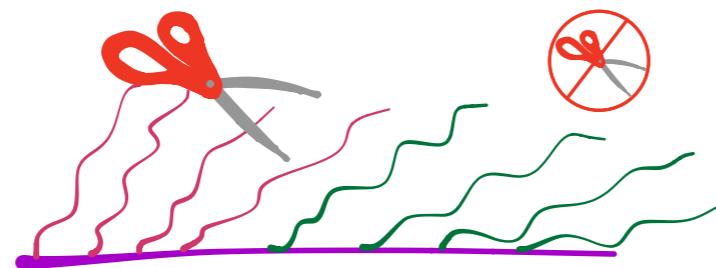
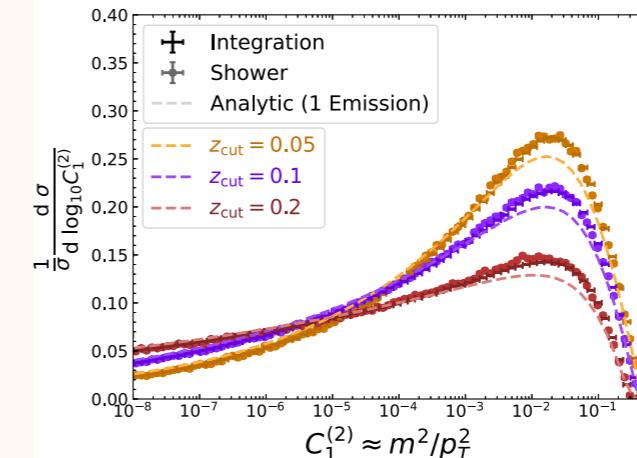
Recursive Safe Subtraction: tree-based approx. to optimal transport grooming

Fixed coupling, **multiple emission** calculations:

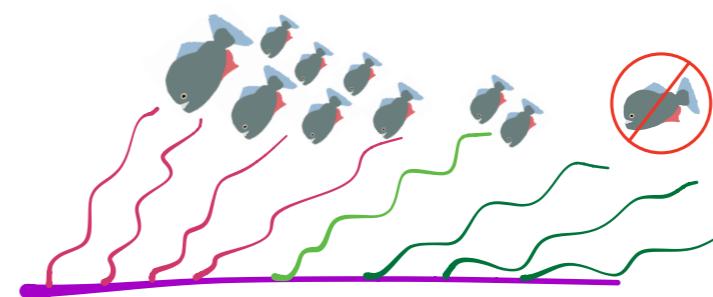
## Soft Drop/mMDT



## PIRANHA-RSS ( $f = 1$ )



Sharp cutoff → kink



No sharp cutoff → smooth

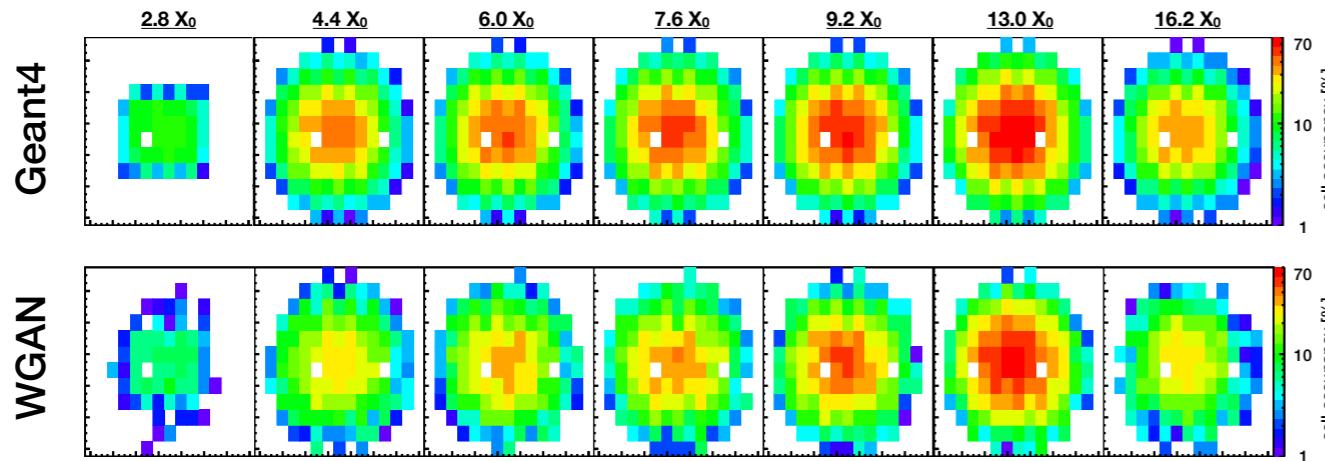
[Slides from Sam Alipour-fard]

[Alipour-fard, Komiske, Metodiev, JDT, in progress]



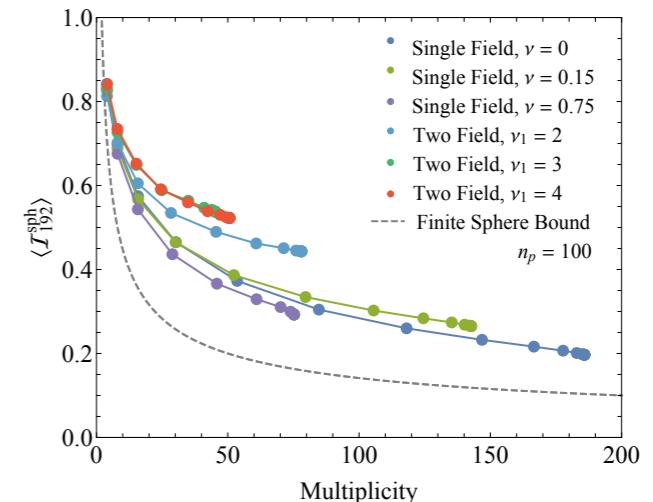
# Wasserstein in HEP

## Generative Modeling



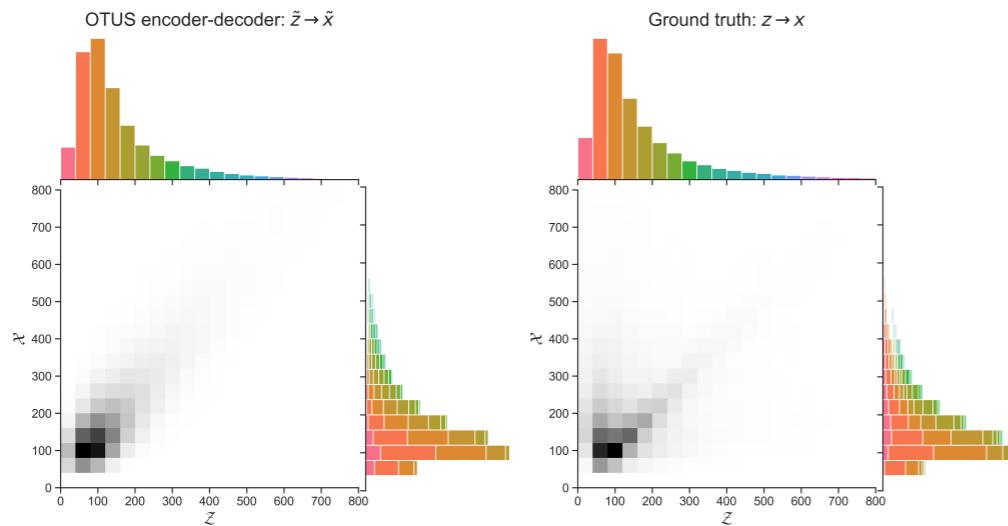
[Erdmann, Geiger, Glombitza, Schmidt, [CSBS 2018](#); Erdmann, Glombitza, Quast, [CSBS 2019](#);  
Chekalina, Orlova, Ratnikov, Ulyanov, Ustyuzhanin, Zakharov, [CHEP 2018](#)]

## BSM Characterization



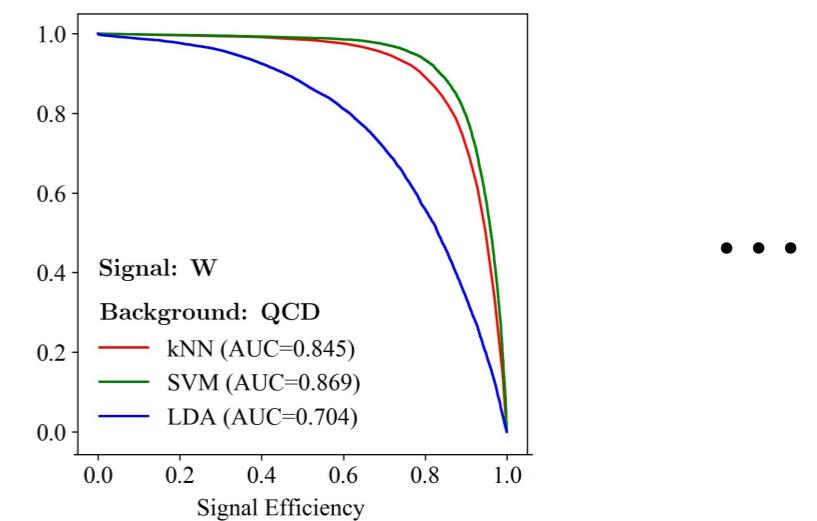
[Cesarotti, Reece, Strassler, [JHEP 2021](#), arXiv 2020]

## Estimated Simulation/Unfolding



[Howard, Mandt, Whiteson, Yang, arXiv 2021]

## Jet Classification



[Cai, Cheng, Craig, Craig, PRD 2020]