

The Geometry of Particle Collisions: Hidden in Plain Sight

Jesse Thaler



&



(since January 2020)

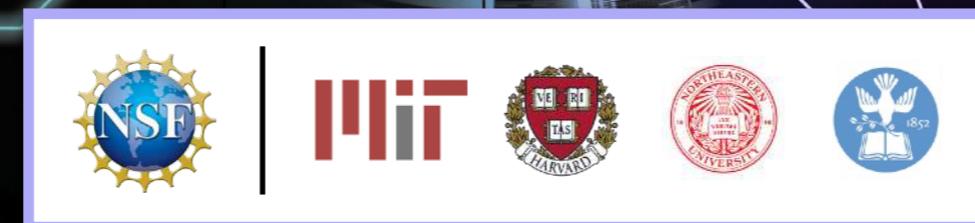
Stochastics and Statistics Seminar, MIT Statistics and Data Science Center — December 3, 2021

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

“eye-phi”



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



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

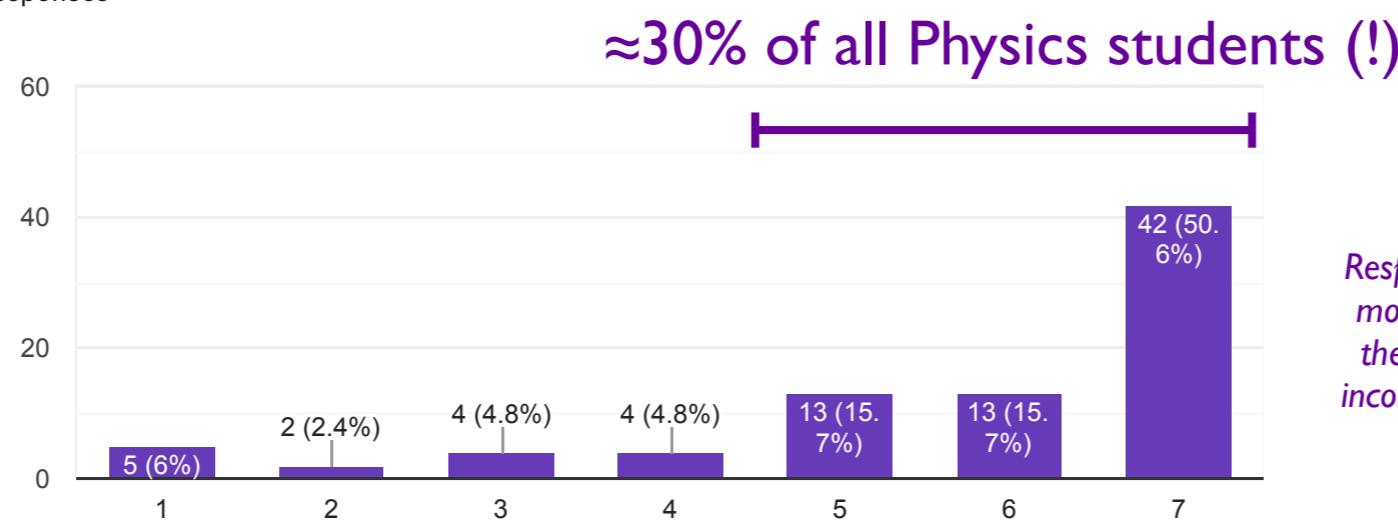
New! PhD in Physics, Statistics & Data Science

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

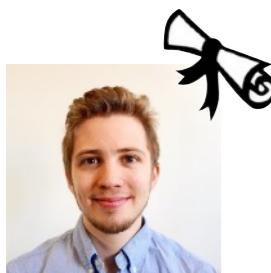


How interested would you be in submitting and defending a PhD thesis that uses statistical methods in a substantial way?

83 responses



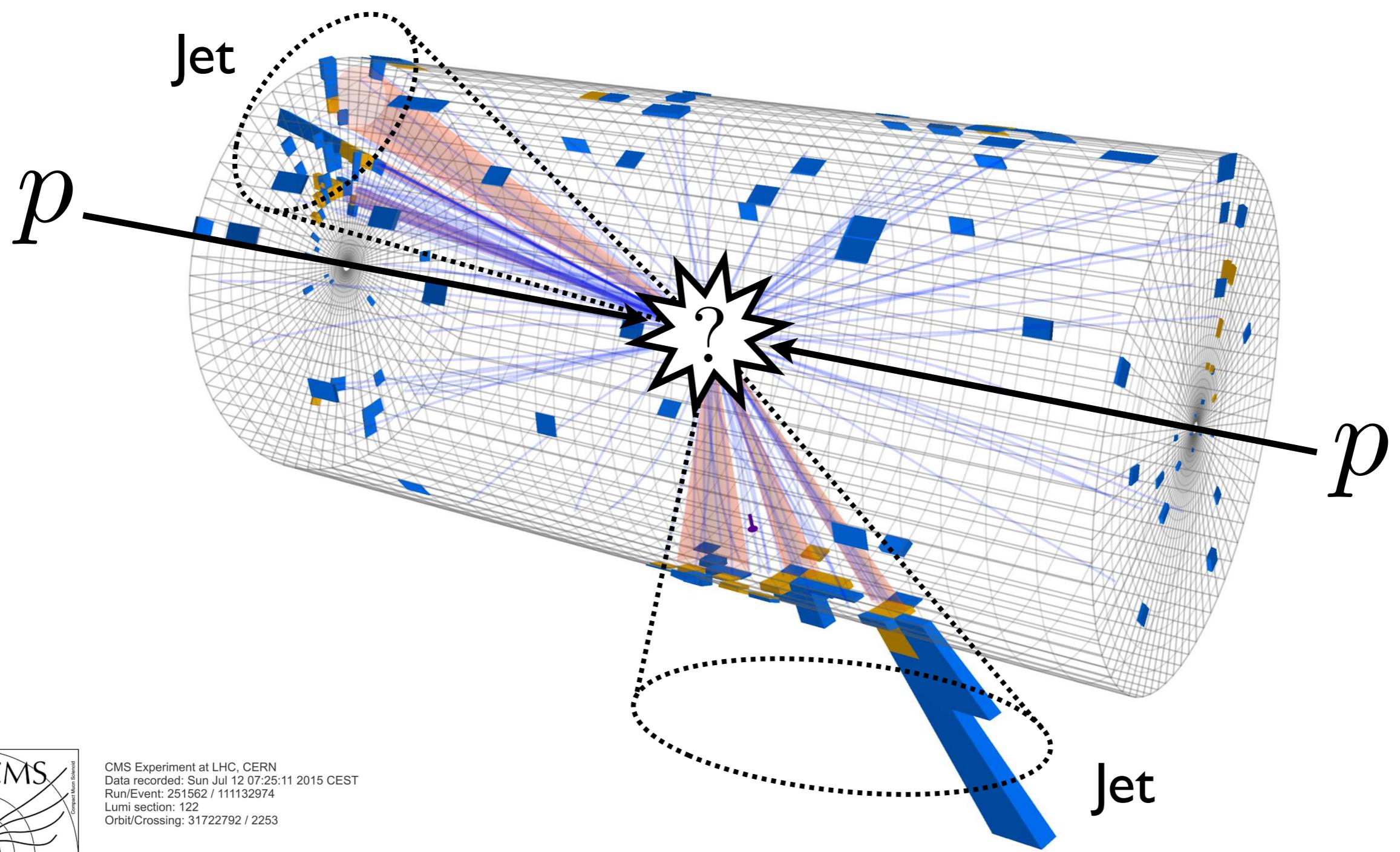
Respondent #11: “I think ML is the most important thing happening in the world right now and should be incorporated into any STEM degree.”



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

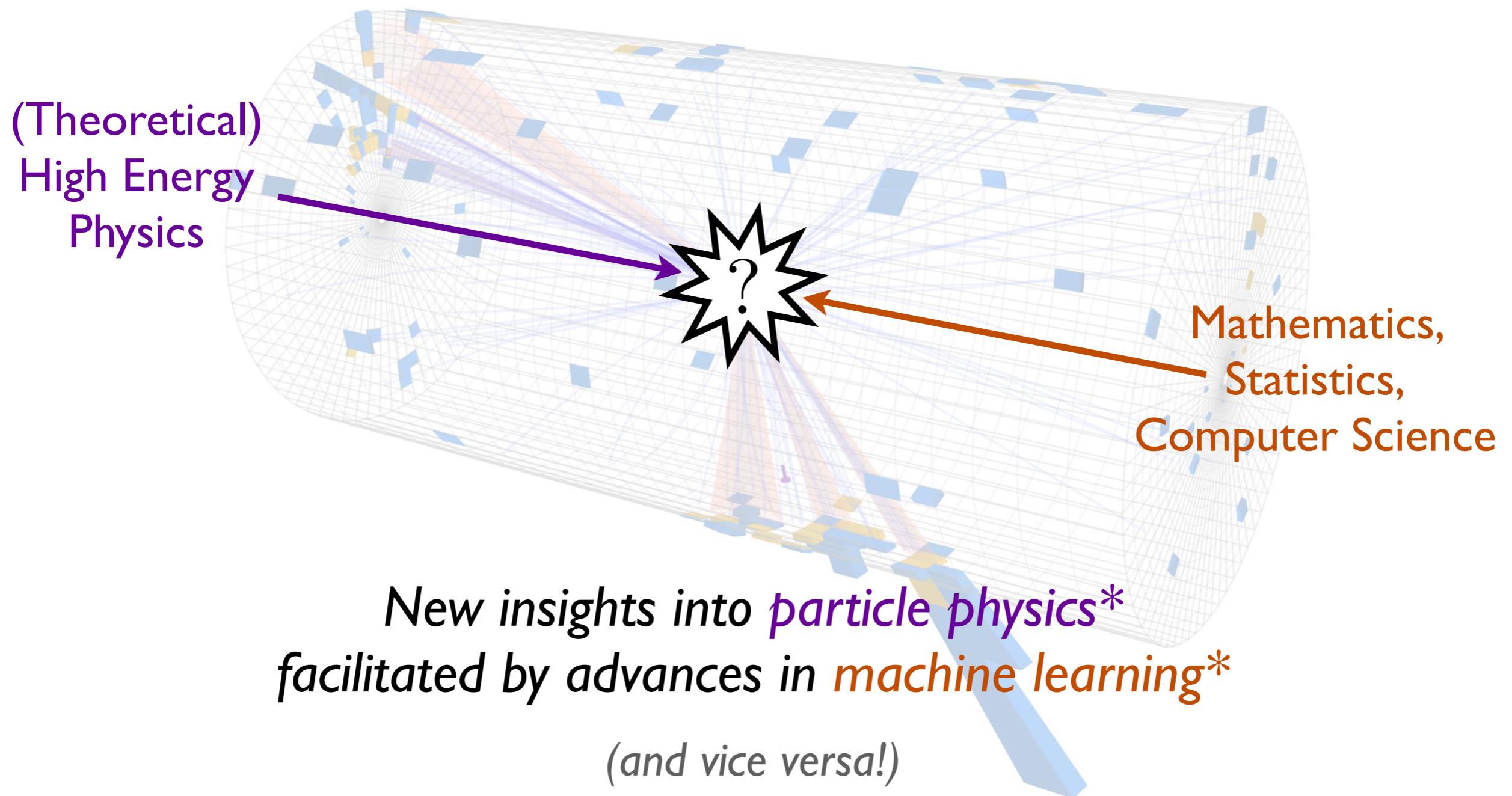
[<https://physics.mit.edu/academic-programs/graduate-students/psds-phd/>]

“Collision Course”



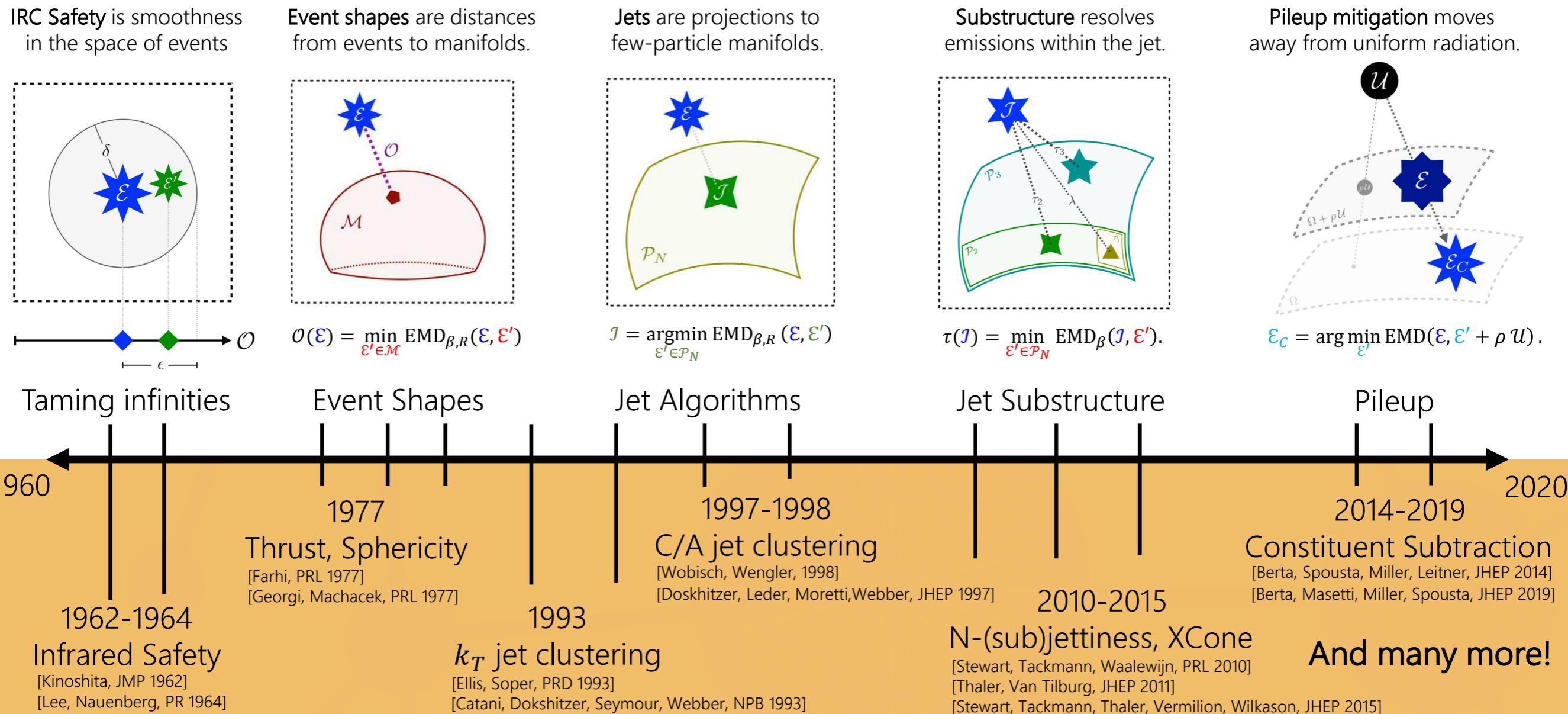
“Collision Course”

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



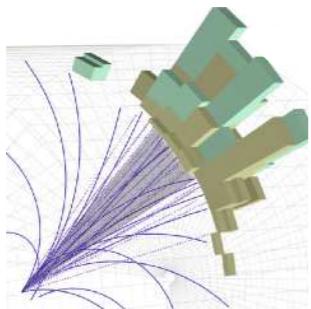
Today: Hidden in “Plane” Sight

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

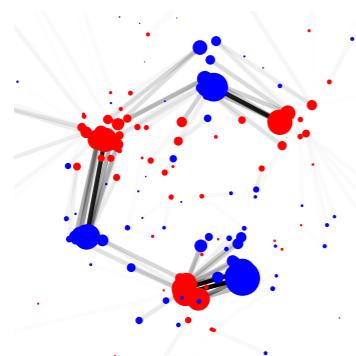


[Komiske, Metodiev, JDT, JHEP 2020; timeline from Metodiev]

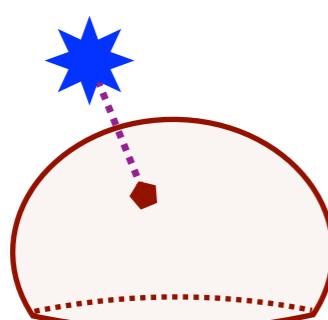
Outline



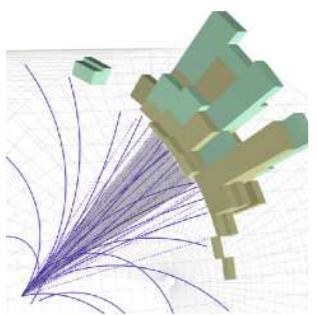
Going with the (Energy) Flow



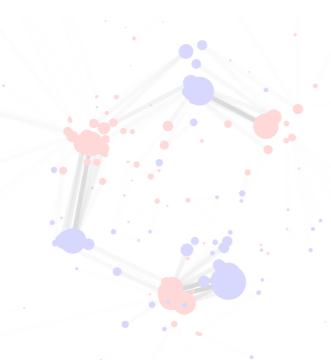
The Energy Mover's Distance



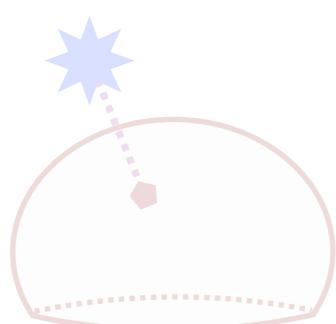
Revealing a Hidden Geometry



Going with the (Energy) Flow

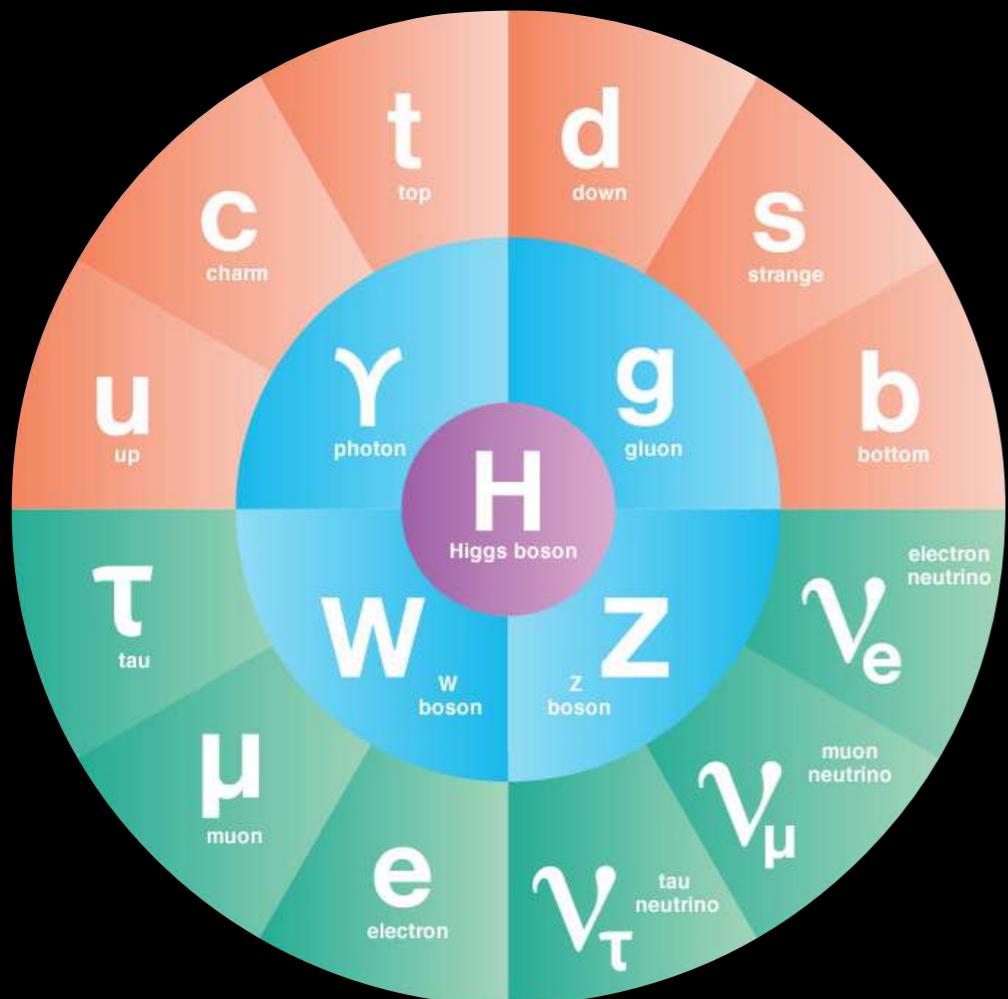


The Energy Mover's Distance

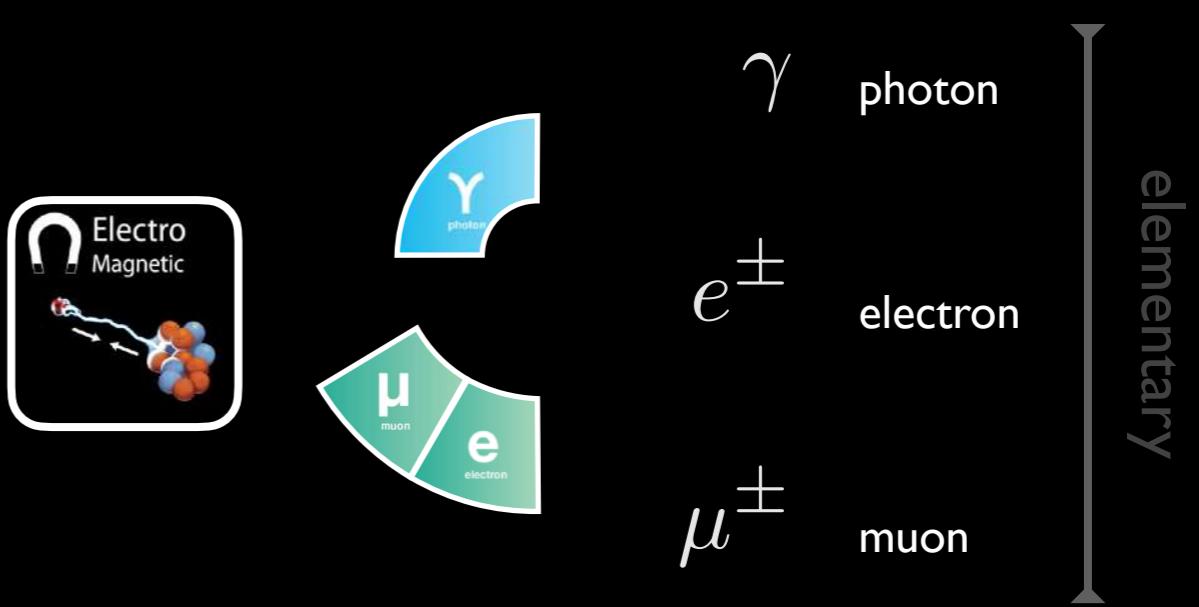
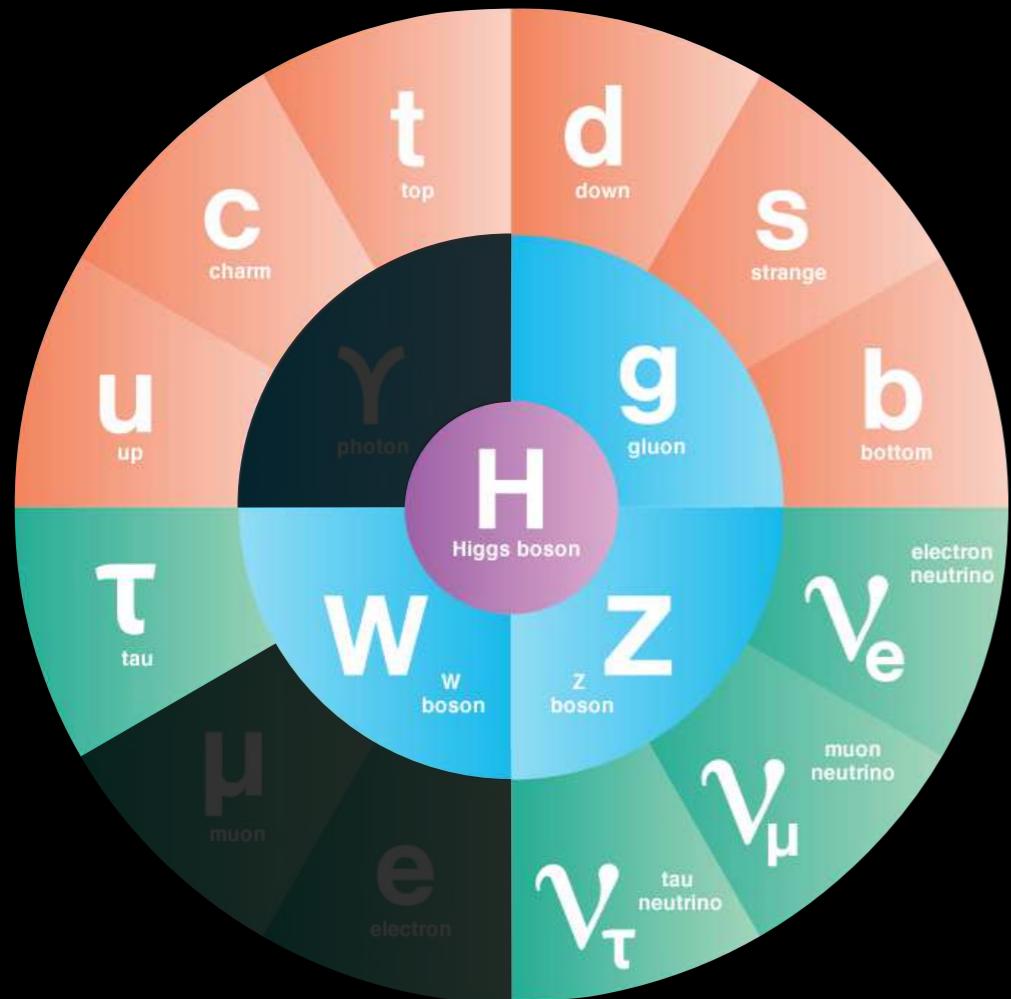


Revealing a Hidden Geometry

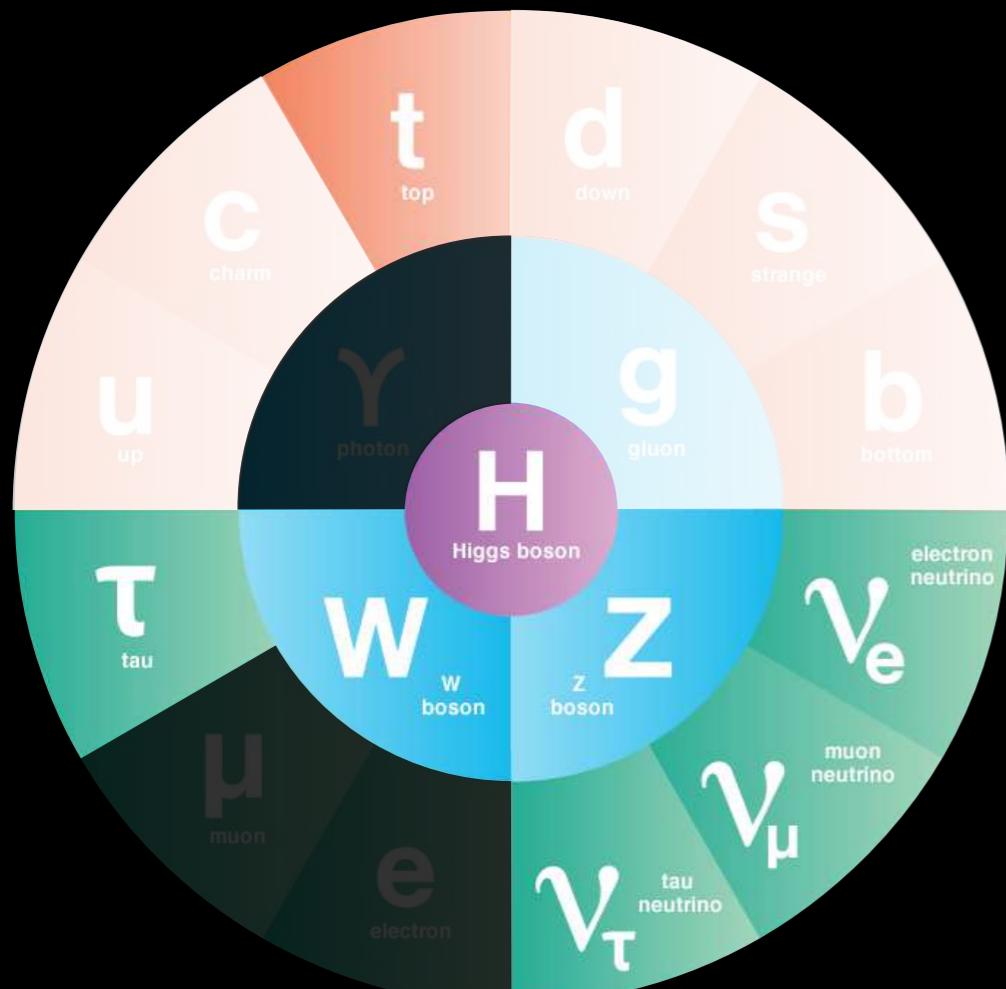
Particle Physics 101



Particle Physics 101

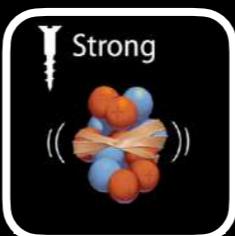


Particle Physics 101



QCD Confinement

Quarks
&
Gluons



γ photon

e^+ electron

μ^+ muon

π^+ pion

K^+ kaon

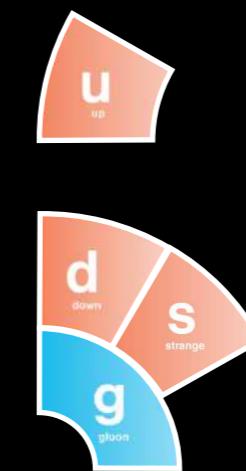
K_L^0 K-long

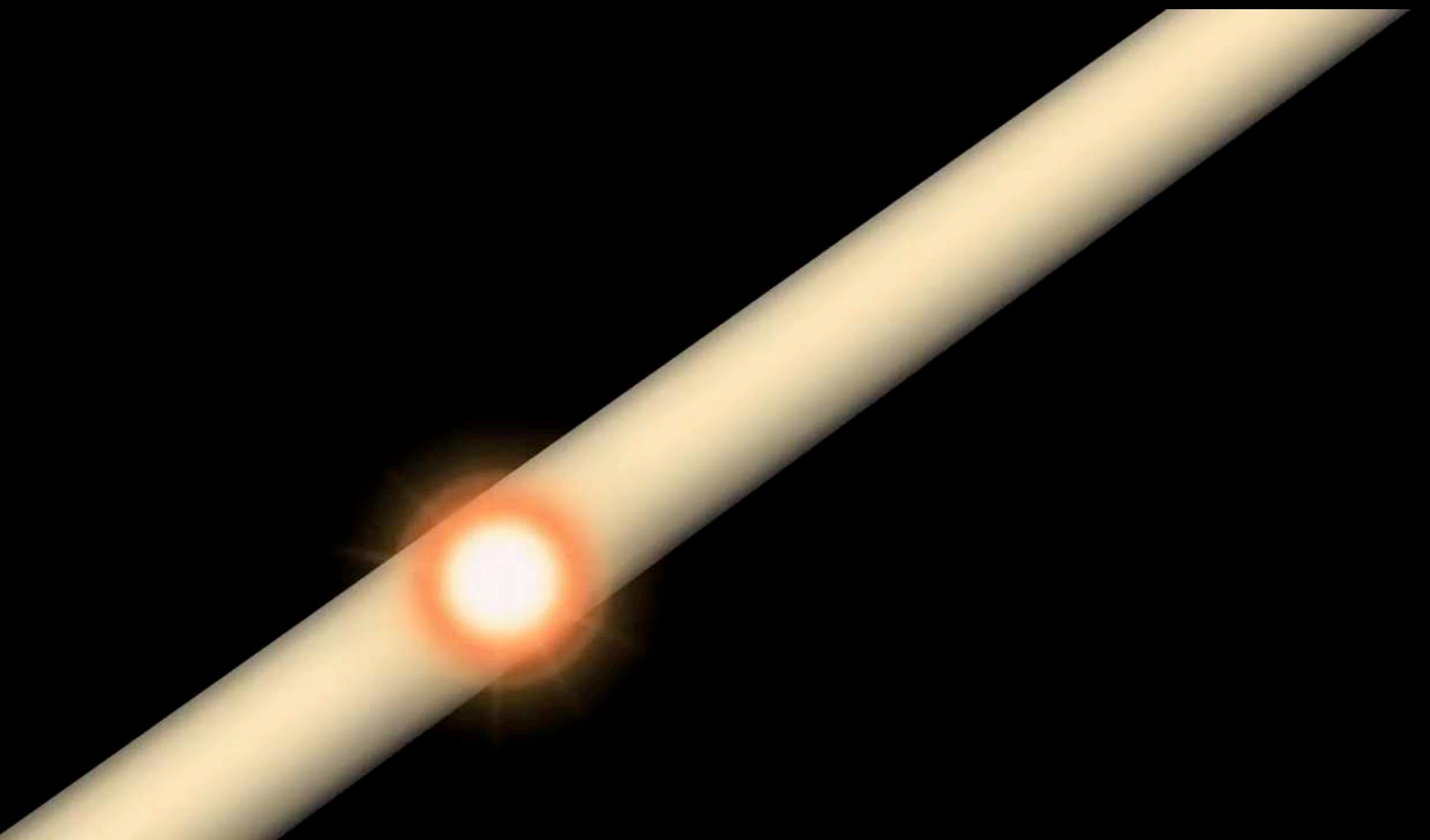
p/\bar{p} proton

n/\bar{n} neutron

elementary

composite



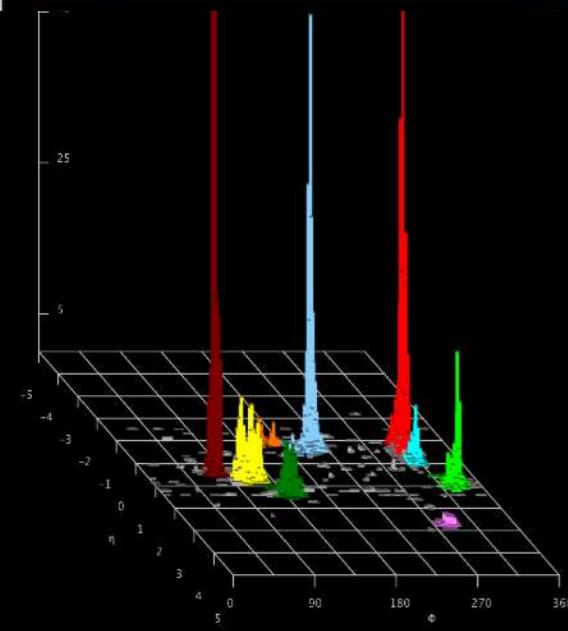
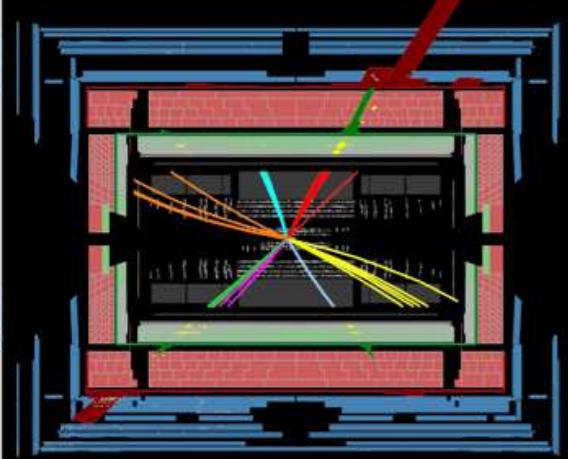




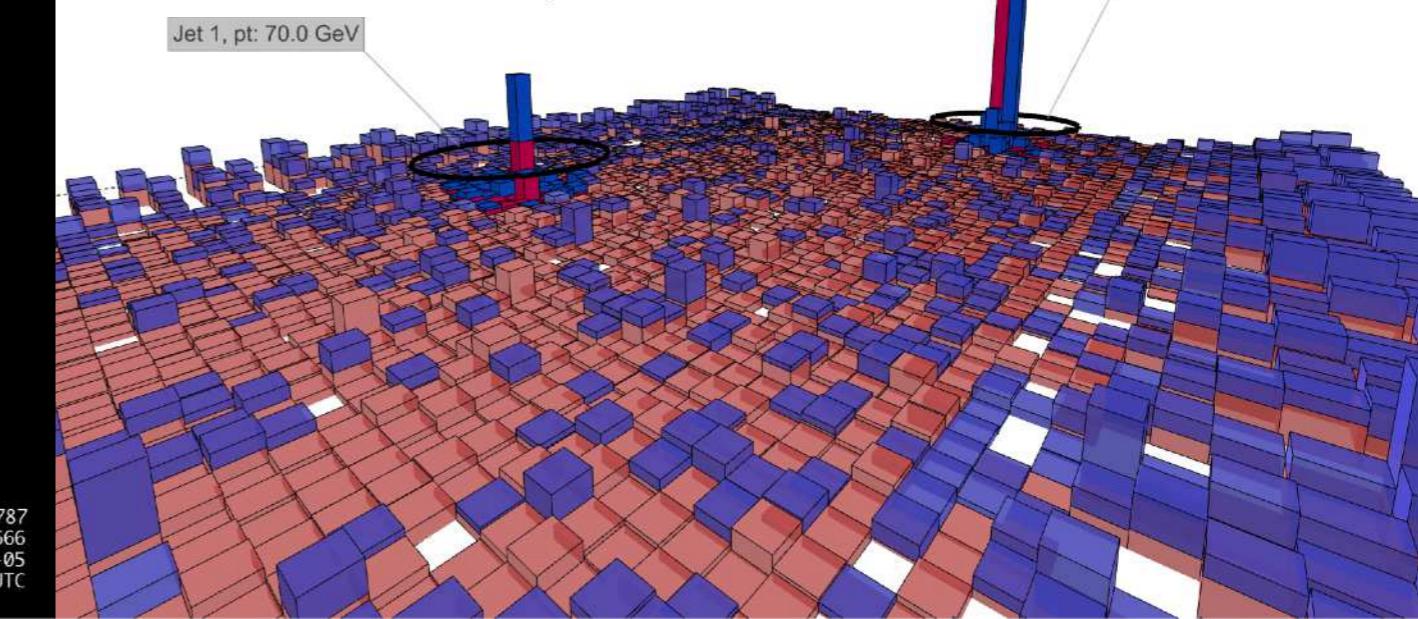
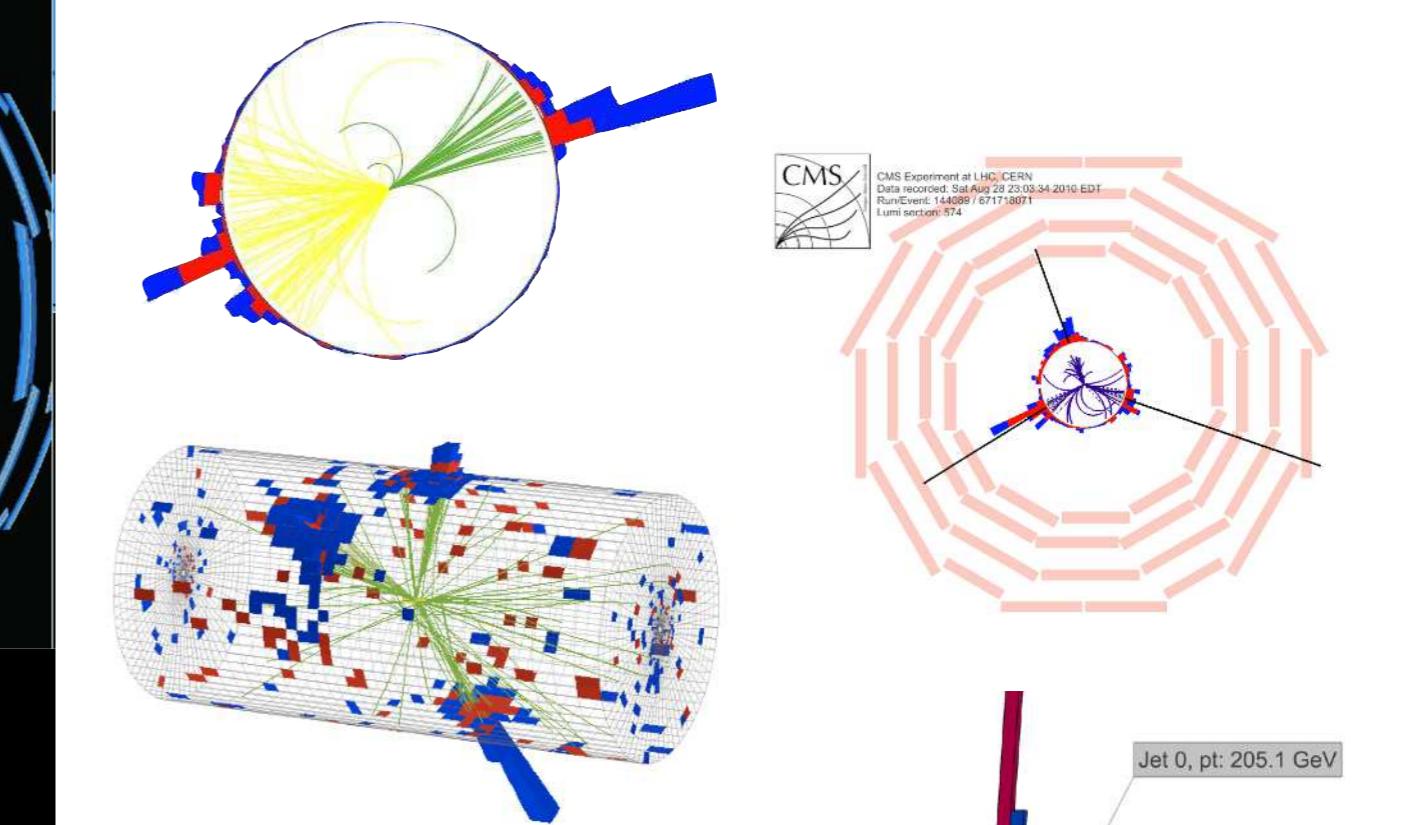
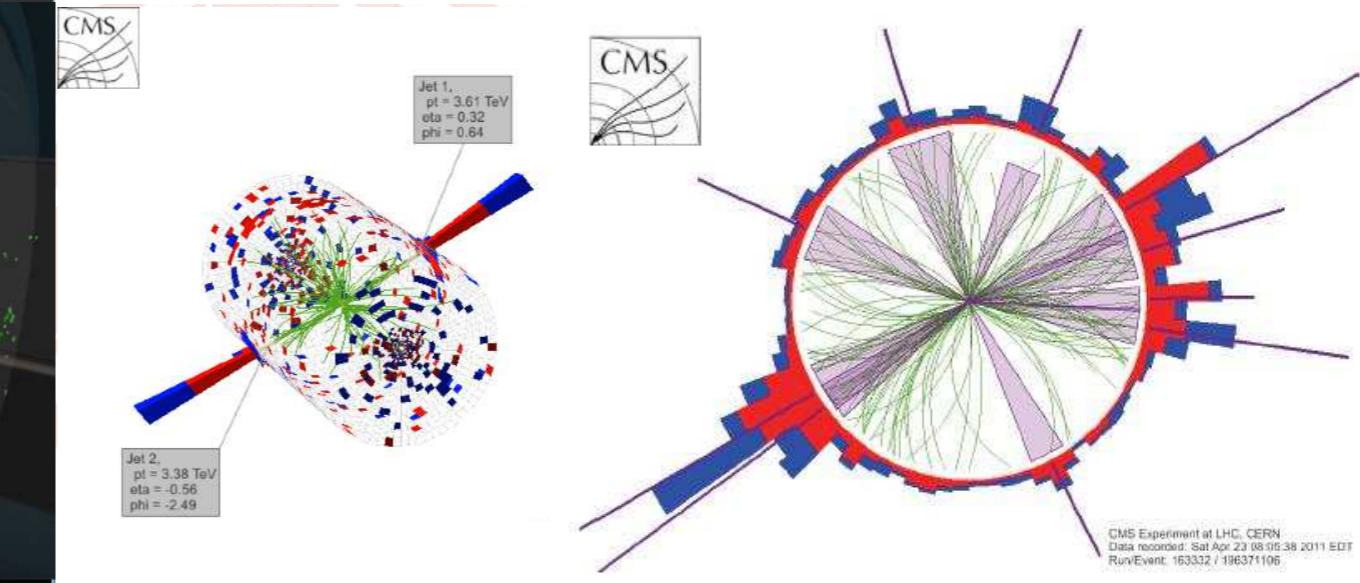
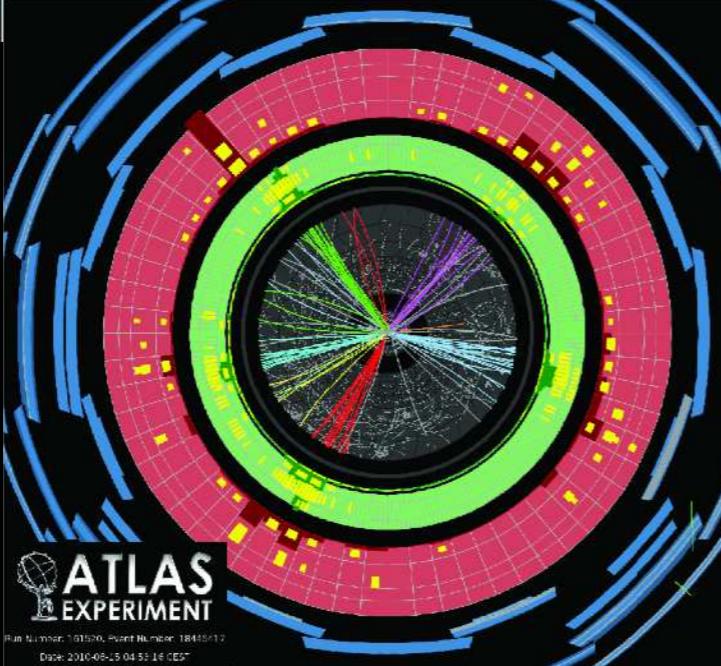
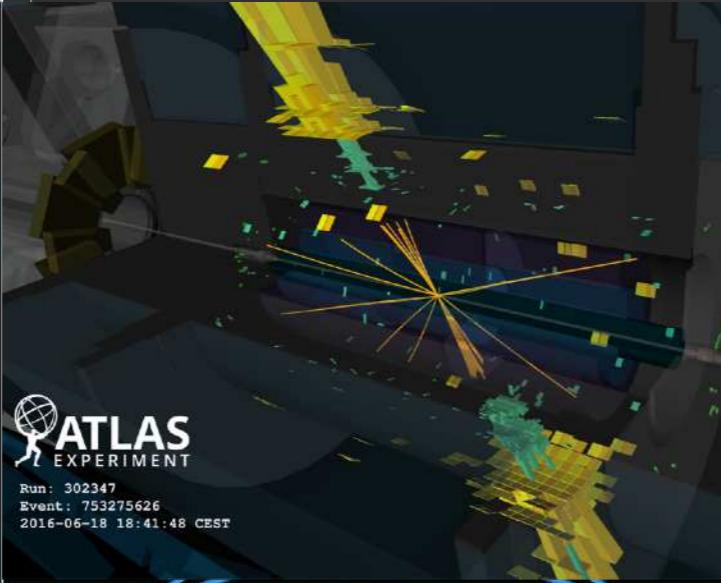
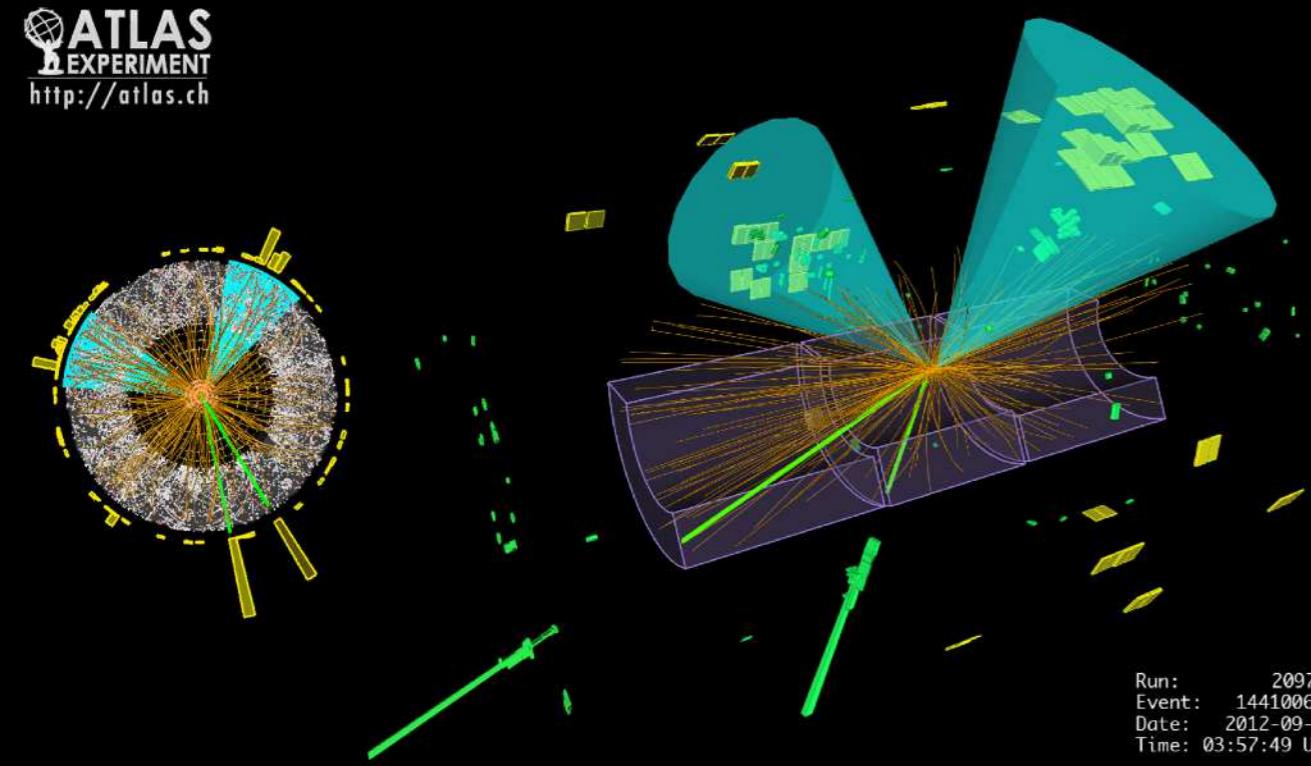


Run Number: 159224, Event Number: 3533152

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

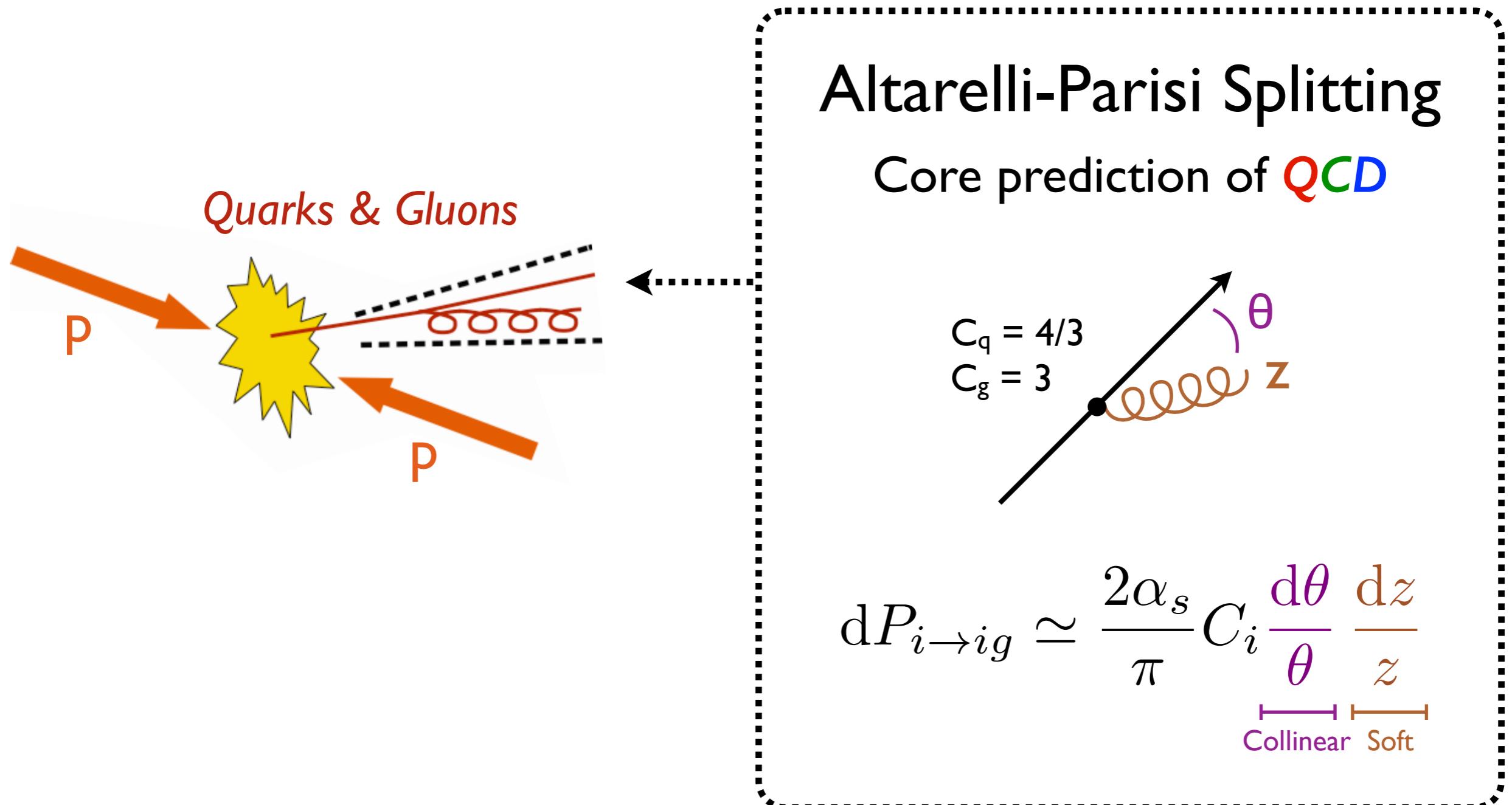


ATLAS
EXPERIMENT
<http://atlas.ch>



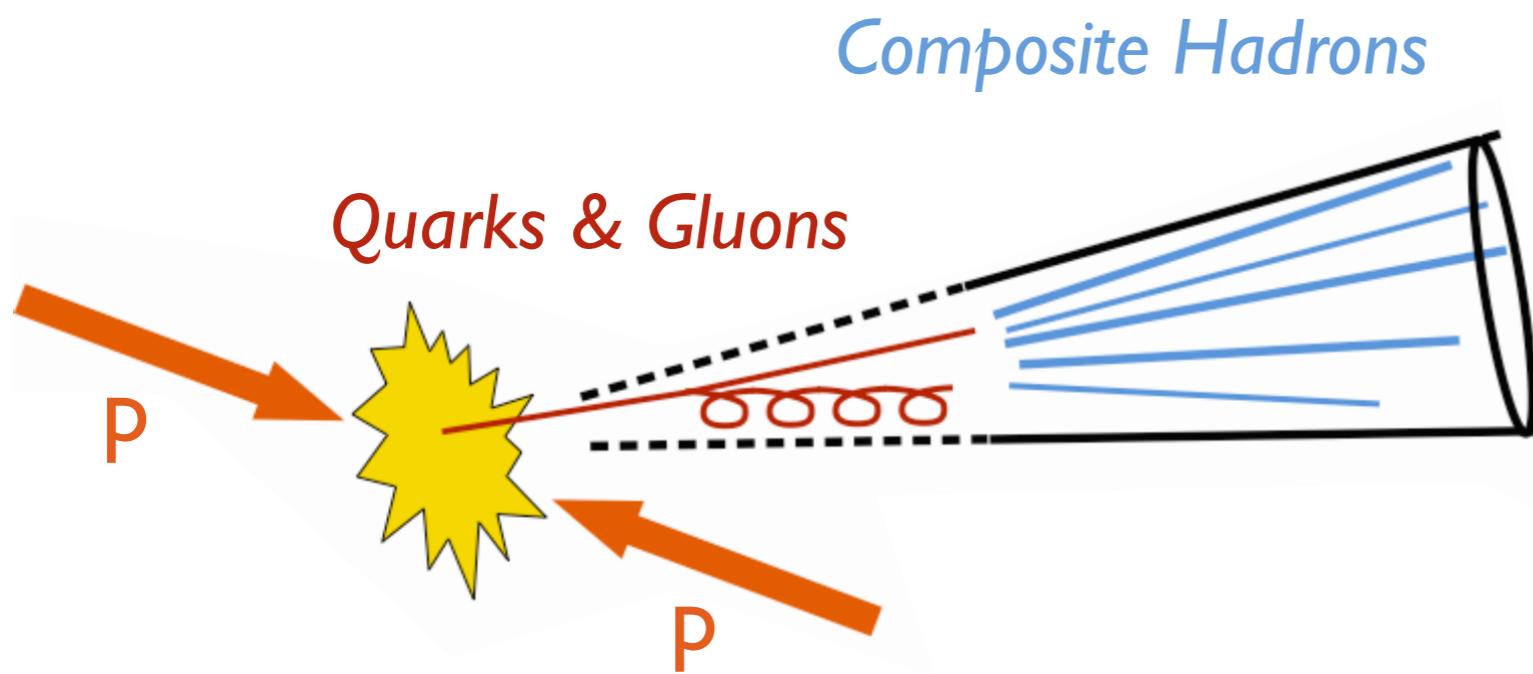
Energy Flow Representation

Emphasizes *infrared and collinear safety*



Energy Flow Representation

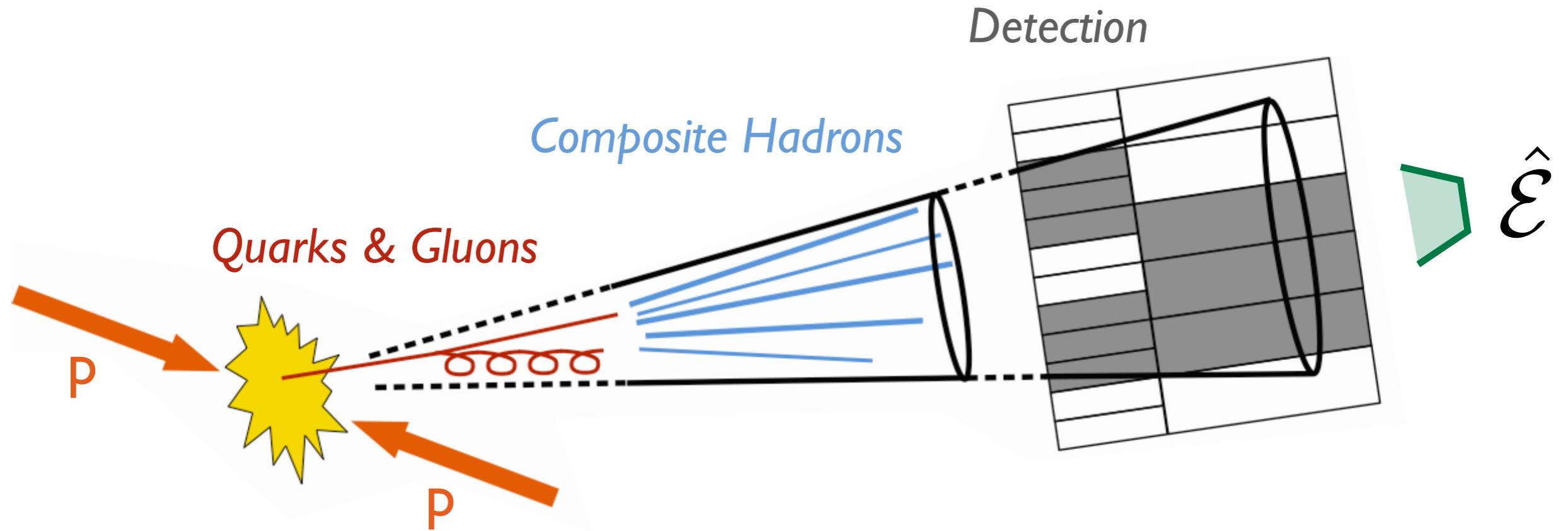
Emphasizes *infrared and collinear safety*



Energy Flow Representation

Emphasizes *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](#)]

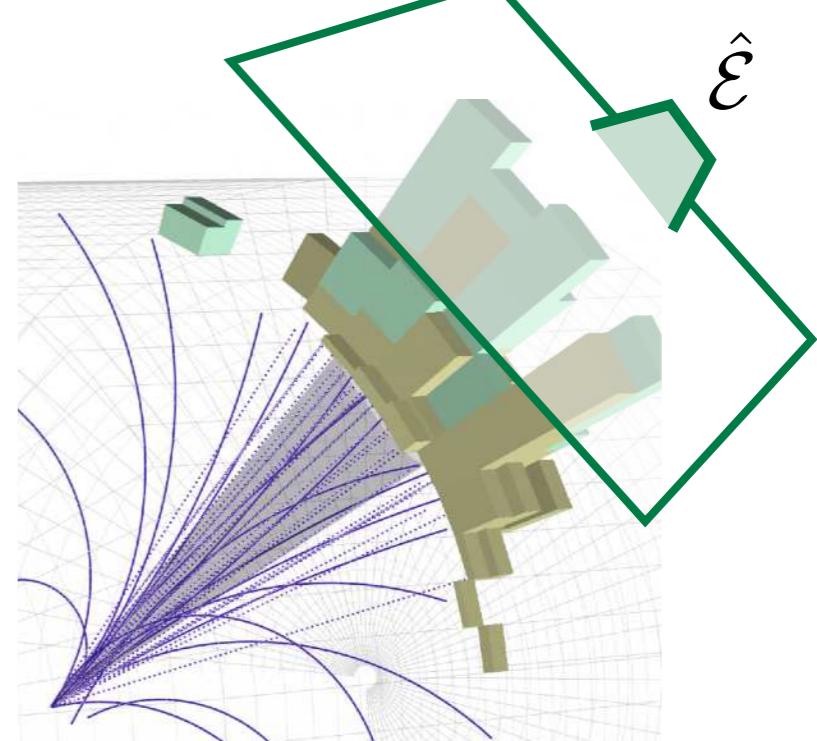
Jets as Weighted Point Clouds

- Energy-Weighted Directions

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

↑ |
Energy Direction

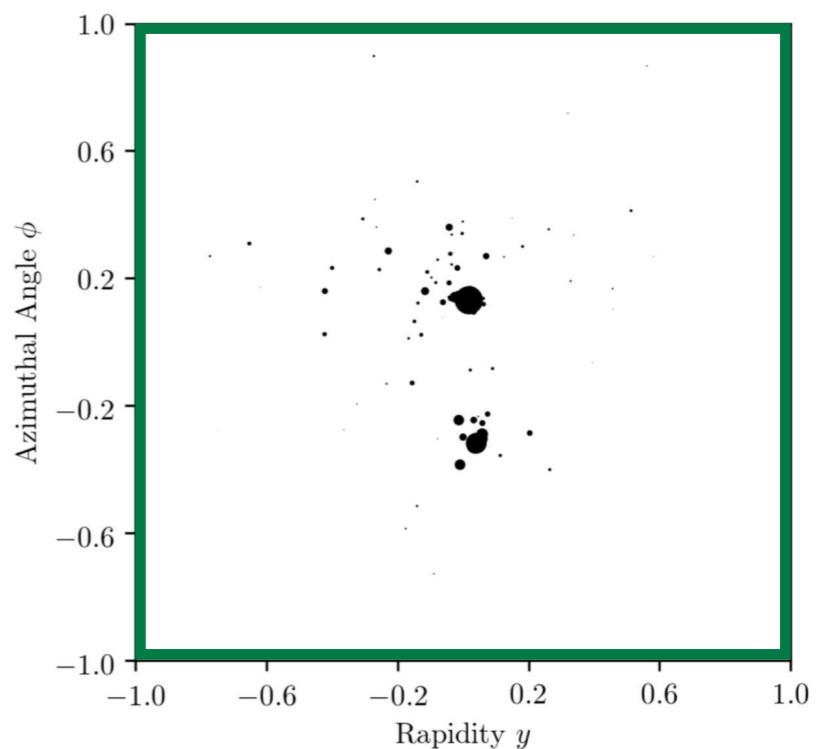
(suppressing “unsafe” charge/flavor information)

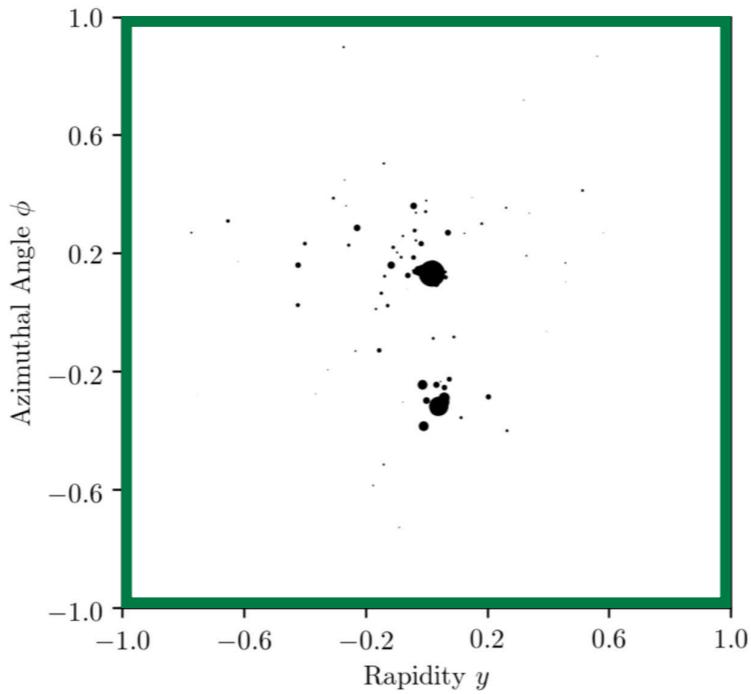


- Equivalently: Energy Density

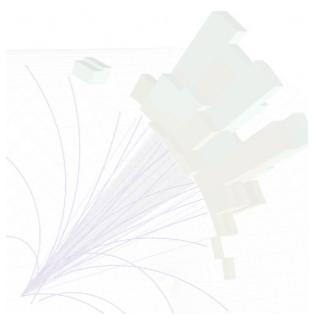
$$\rho(\hat{n}) = \sum_{i \in \mathcal{J}} E_i \delta^{(2)}(\hat{n} - \hat{n}_i)$$

↑ ↑
Energy Direction

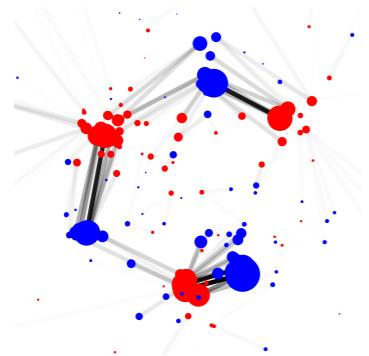




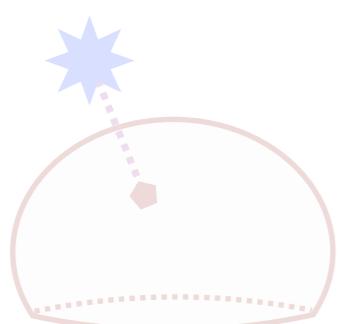
*When restricted to IRC safe information,
jets/events are naturally represented
as **energy densities***



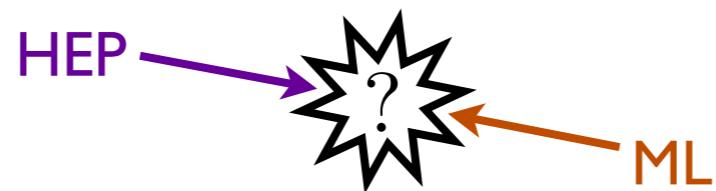
Going with the (Energy) Flow



The Energy Mover's Distance



Revealing a Hidden Geometry



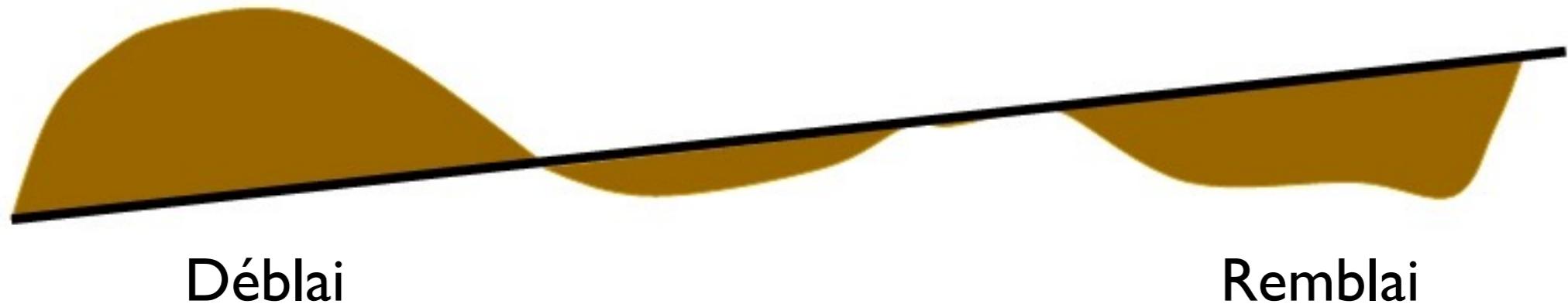
*If you ask your local computational geometry
expert how to process densities...*

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



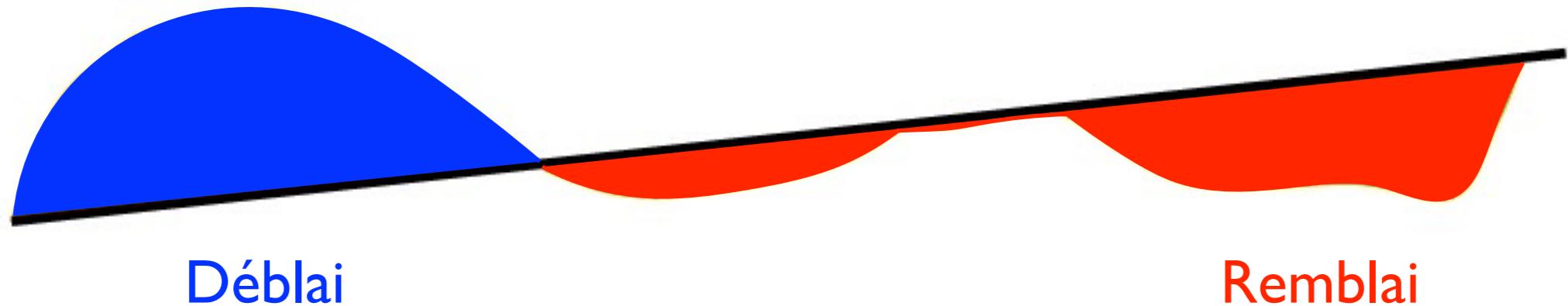
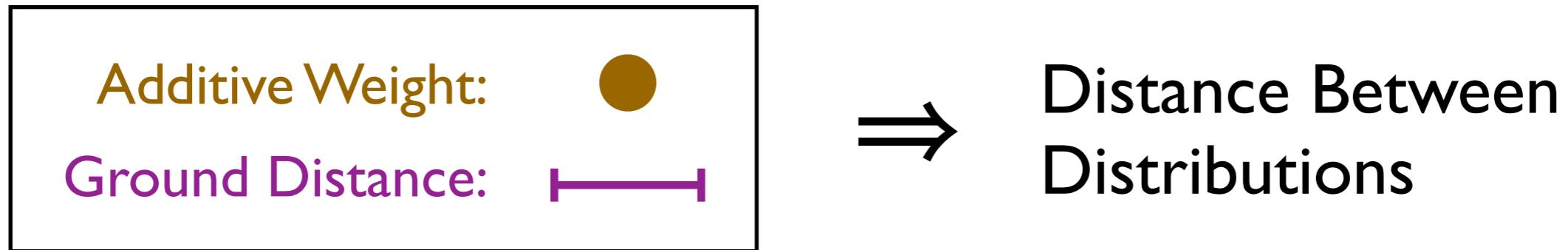
[h/t Niles-Weed, [ML4Jets 2020](#); Monge, 1781; Kantorovich, 1939; Vaserštejn, 1969; [Wikipedia](#)]

The Earth Mover's Distance

Optimal Transport:

[Peleg, Werman, Rom, [IEEE 1989](#);
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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](#)]

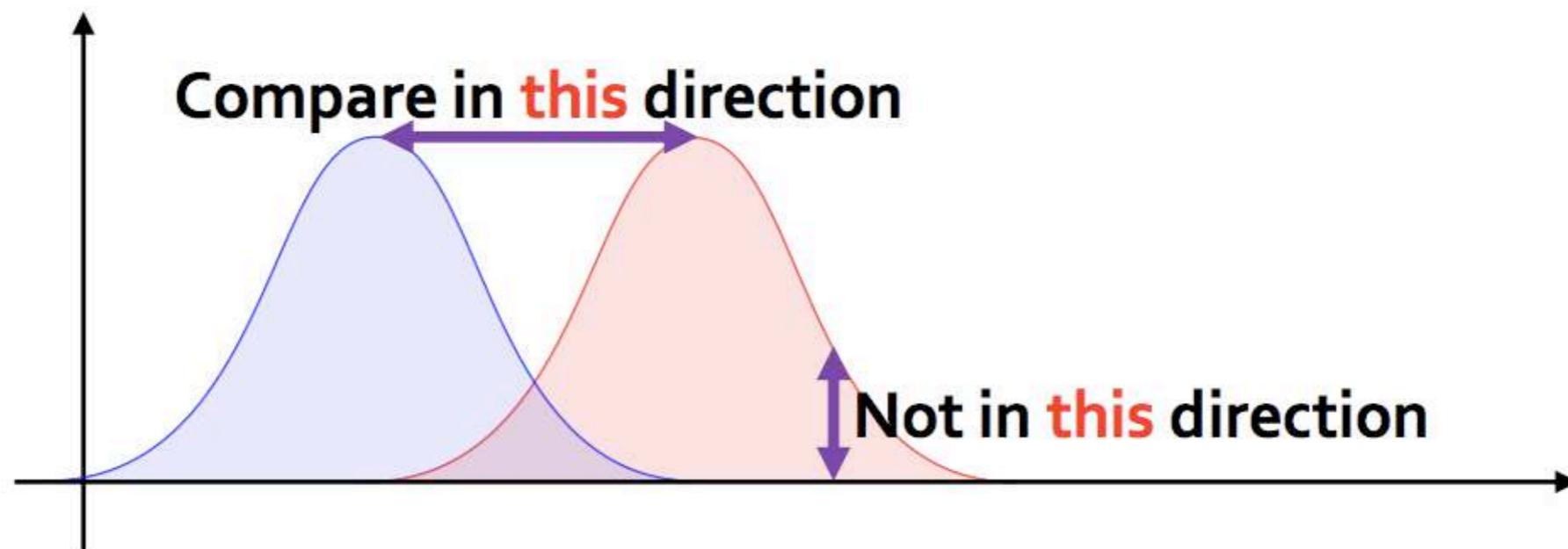
The Earth Mover's Distance

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)

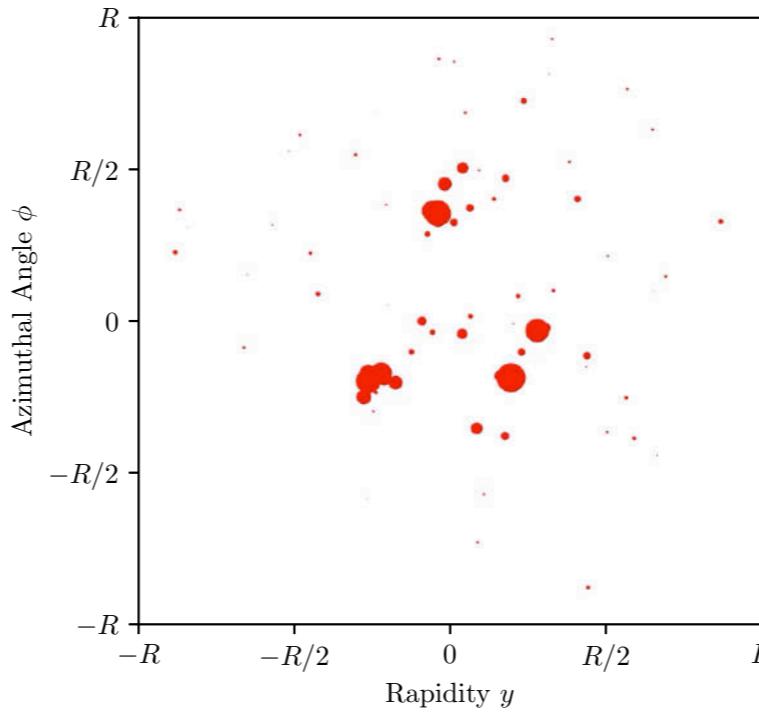


[figure from Kun, [Math n Programming](#)]

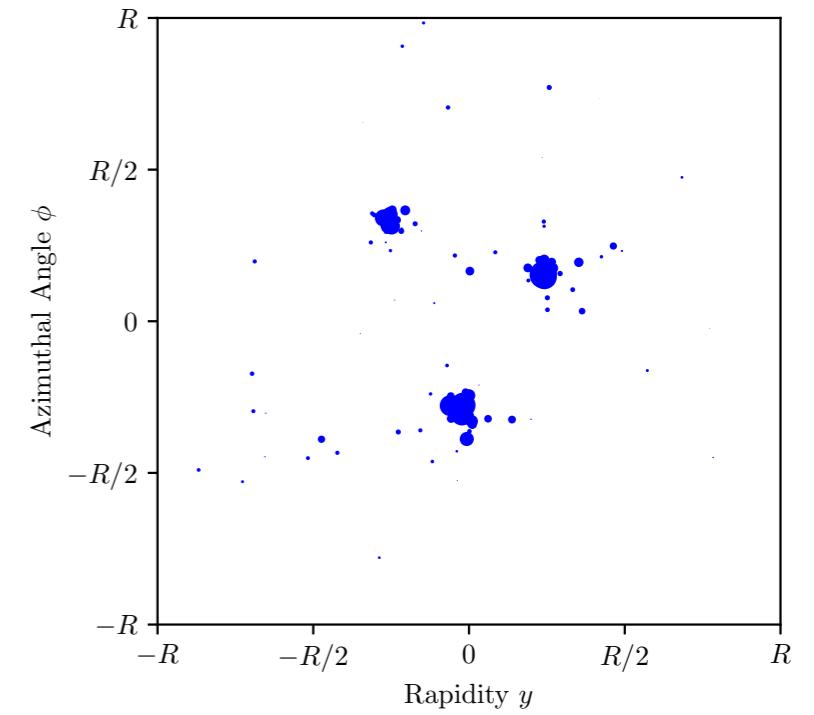
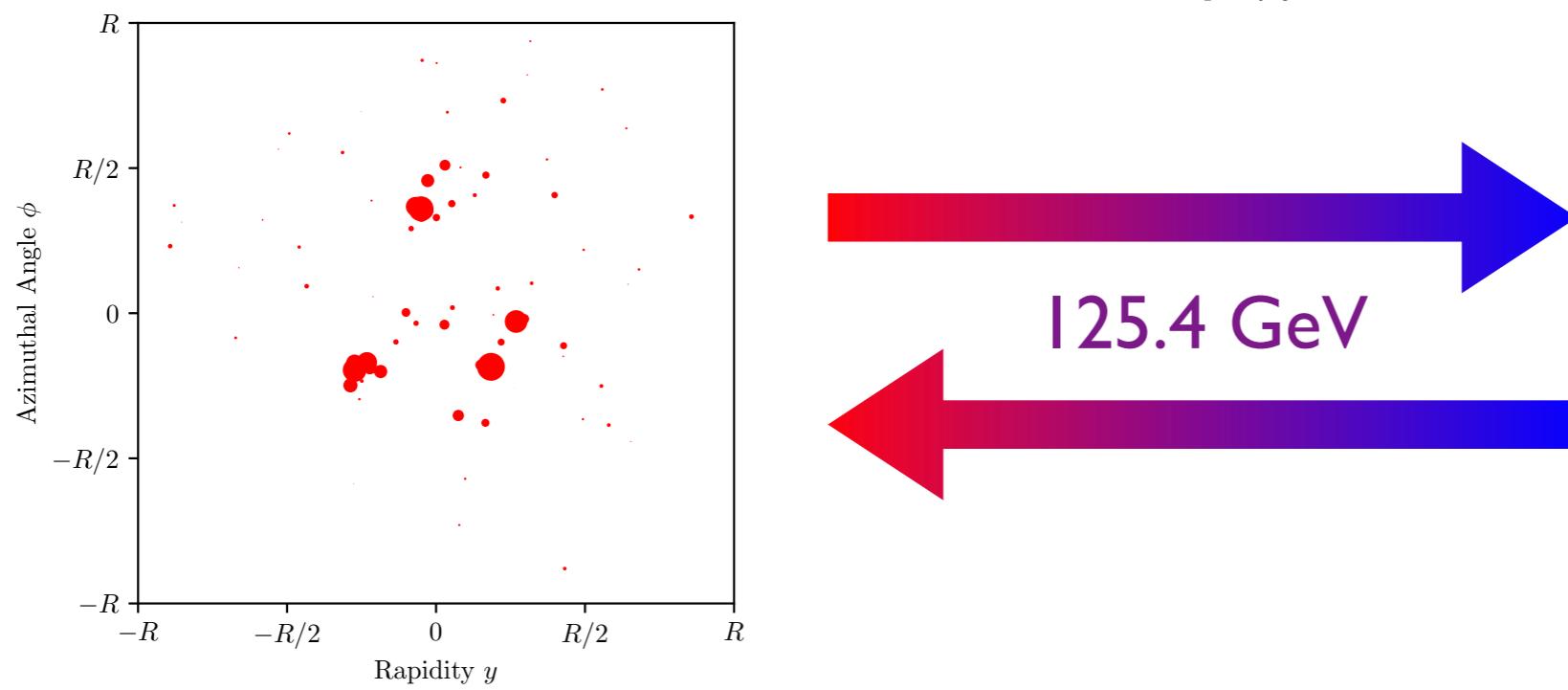
[h/t Niles-Weed, [ML4Jets 2020](#); Monge, 1781; Kantorovich, 1939; Vaserštejn, 1969; [Wikipedia](#)]

Similarity of Two Energy Flows

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

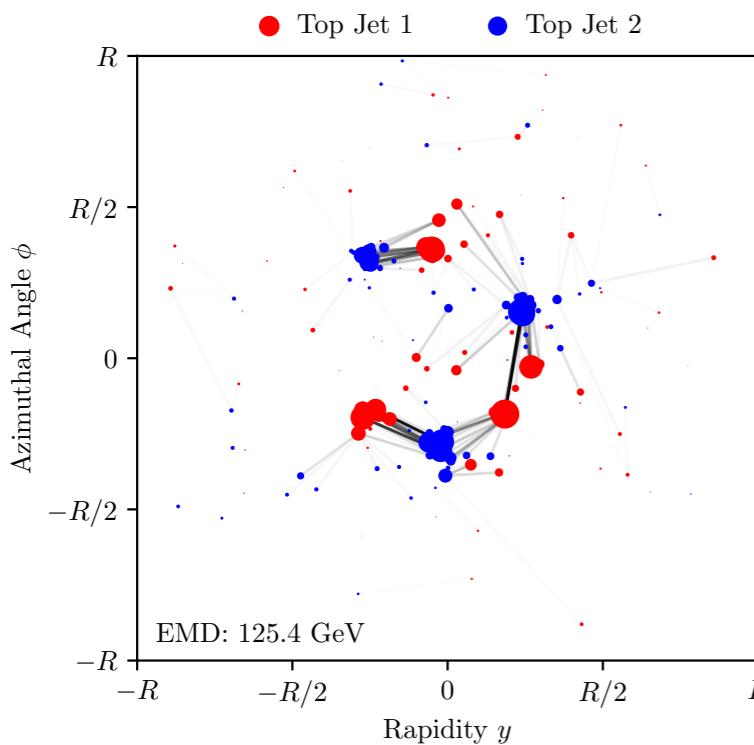
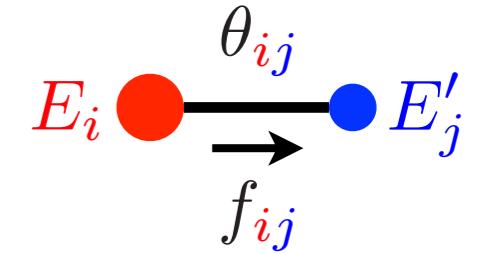


Optimal Transport:
Earth Mover's Distance
a.k.a. l -Wasserstein metric



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

The Energy Mover's Distance



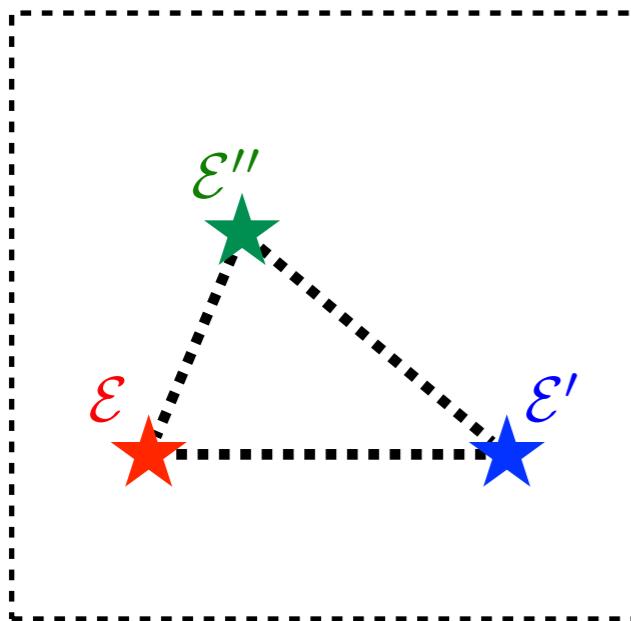
Optimal transport between energy flows...

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

↑
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)

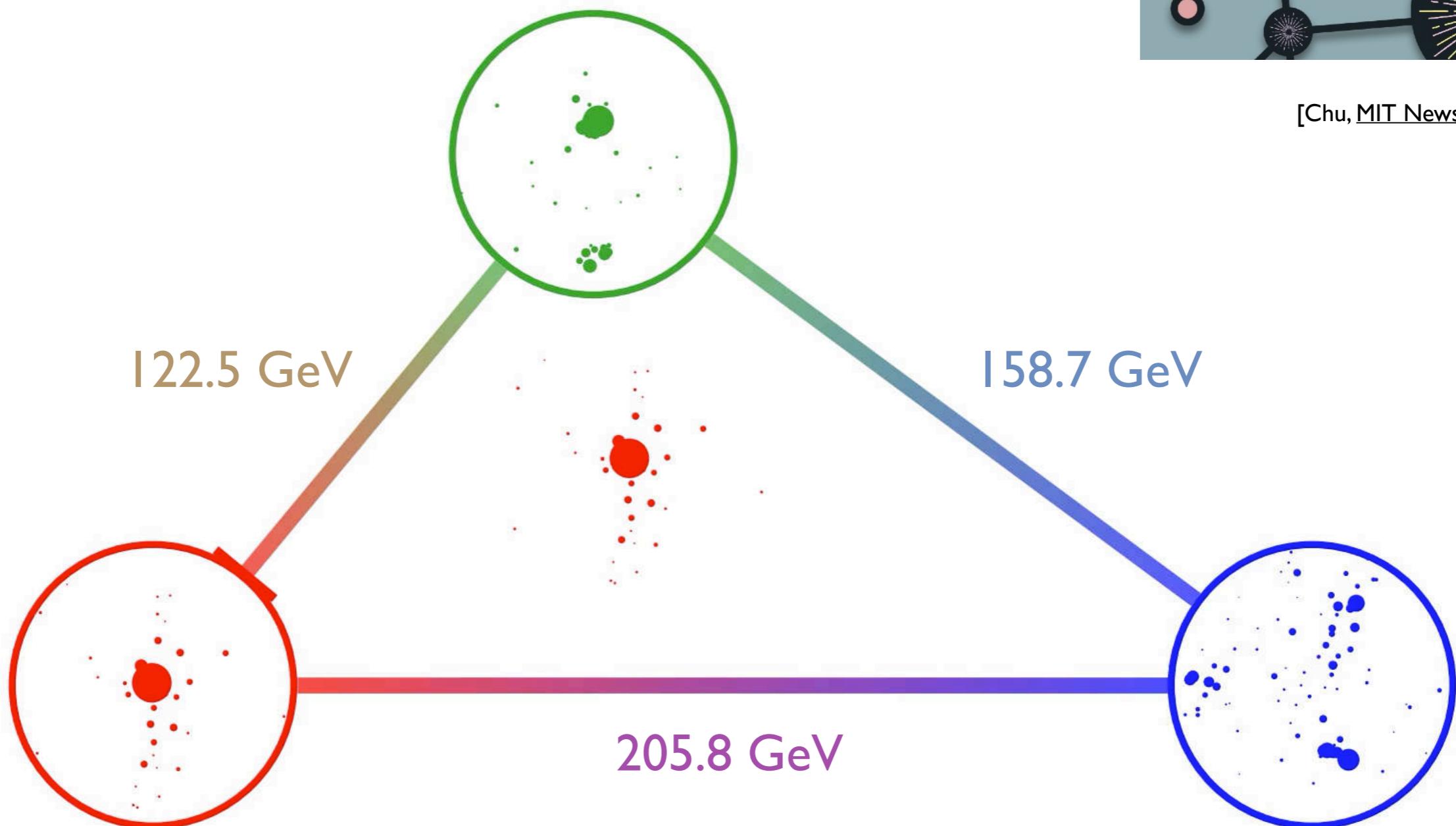
[Komiske, Metodiev, JDT, [PRL 2019](#);
 see also Pele, Werman, [ECCV 2008](#); Pele, Taskar, [GSI 2013](#);
 [see flavored variant in Crispim Romão, Castro, Milhano, Pedro, Vale, [EPJC 2021](#)]
 [see computational speed up in Cai, Cheng, Craig, Craig, [PRD 2020](#)]



Similarity of Three Energy Flows



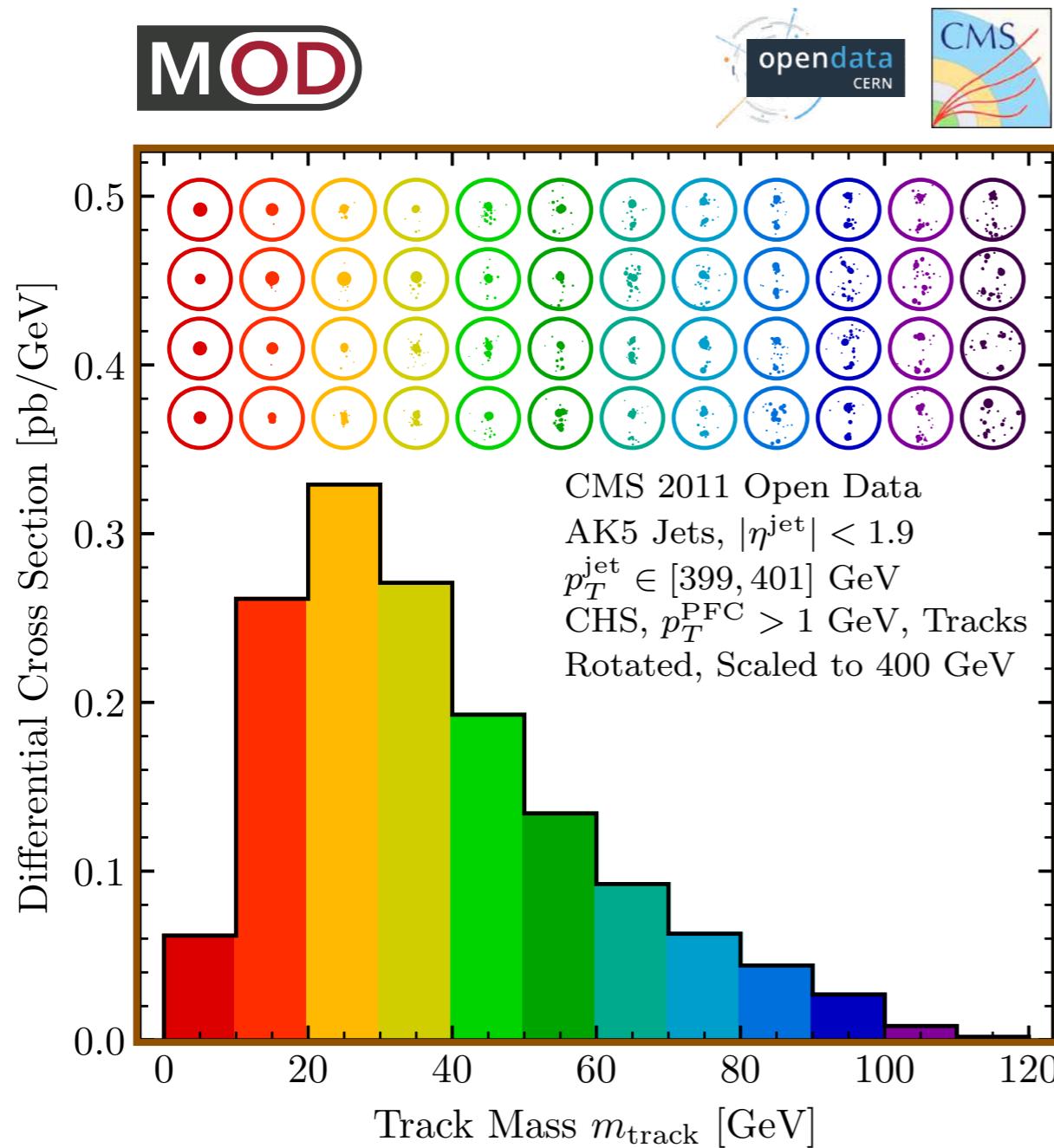
[Chu, MIT News July 2019]



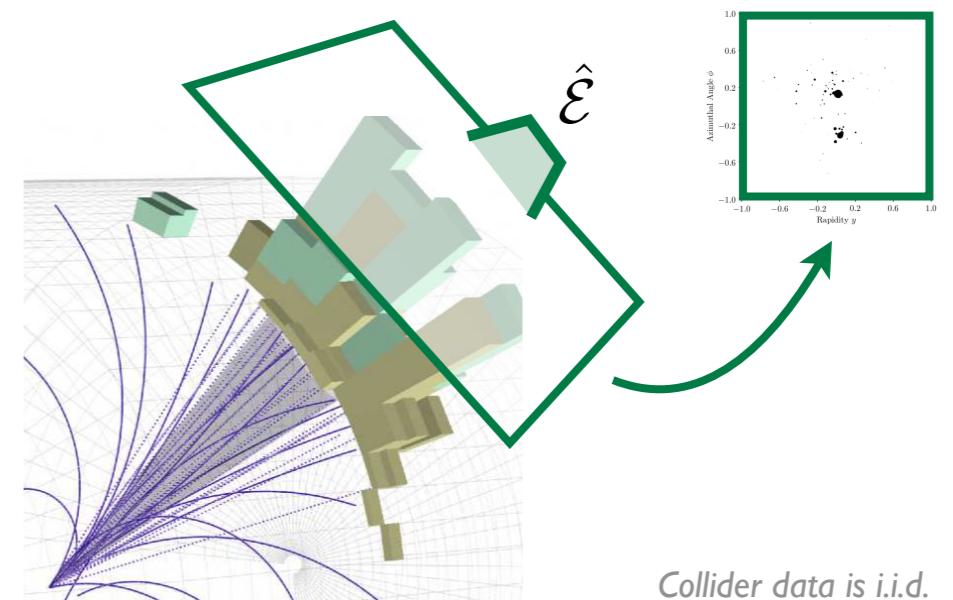
[Komiske, Metodiev, JDT, [PRL 2019](#); code at Komiske, Metodiev, JDT, [energyflow.network](#); see alternative graph network approach in Mullin, Pacey, Parker, White, Williams, [JHEP 2021](#)]



The Forest and the Trees



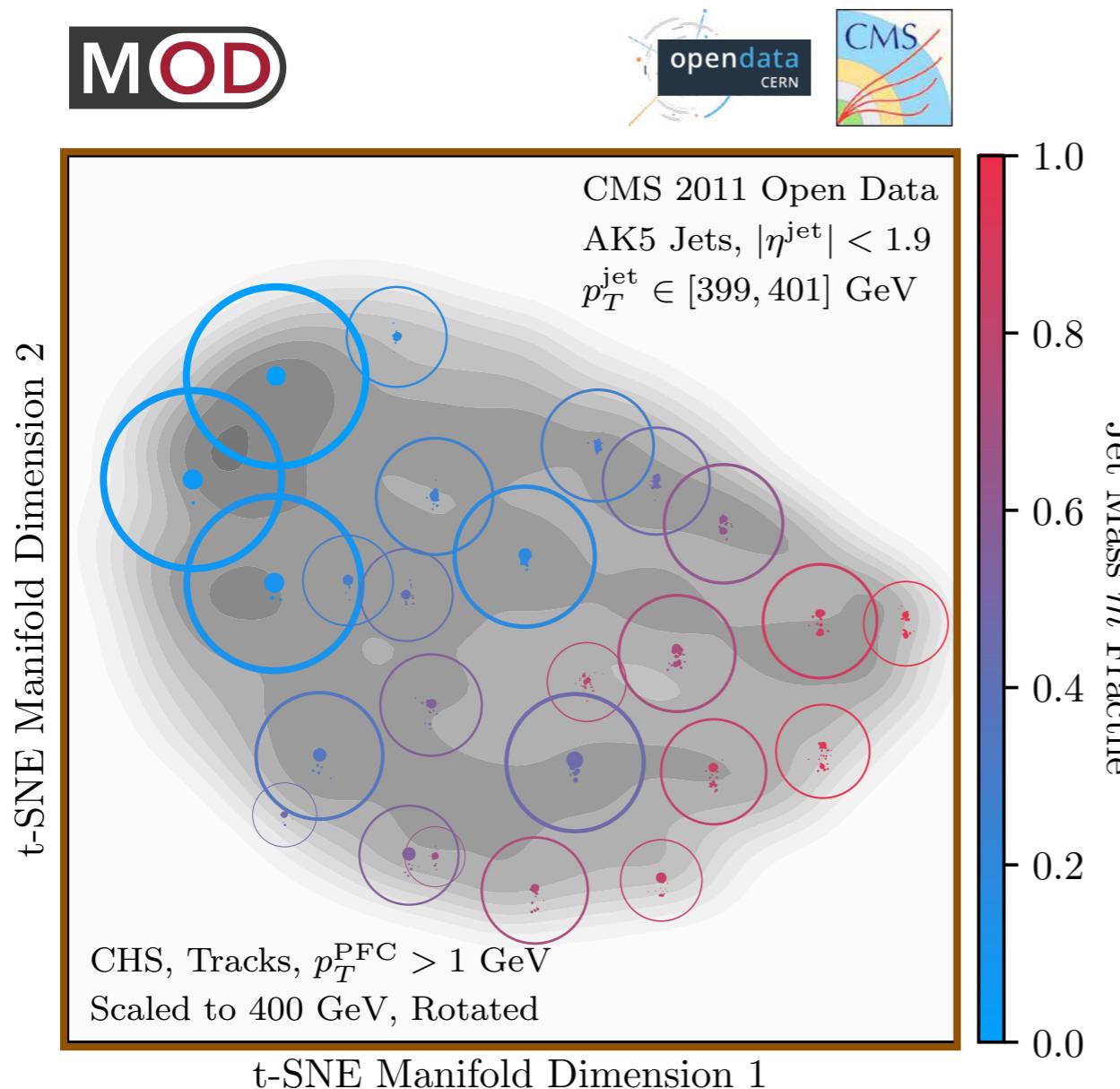
A *Histogram of Observables*



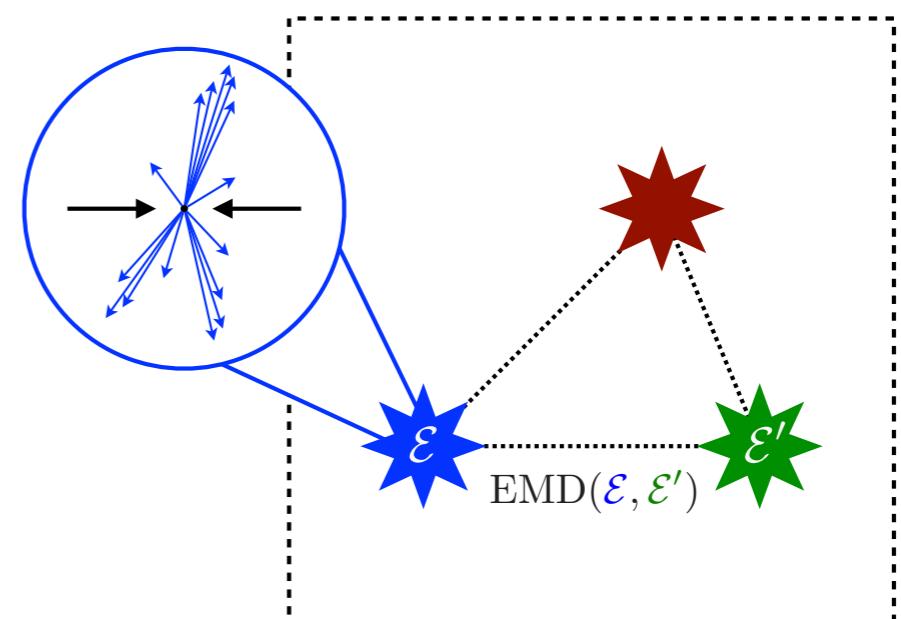
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;
using CMS Open Data]



Building the Forest from the Trees



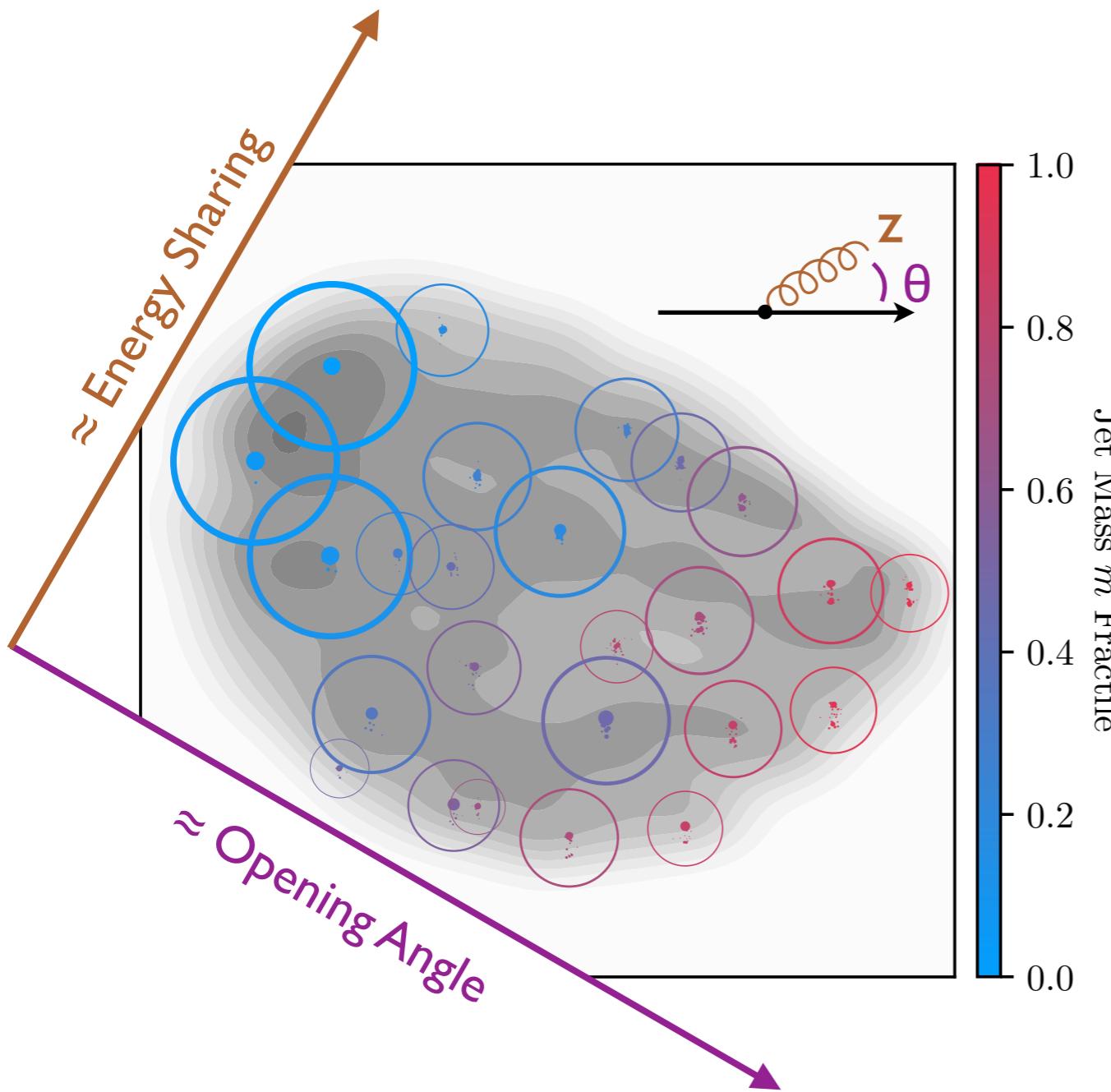
The Space of Energy Flows



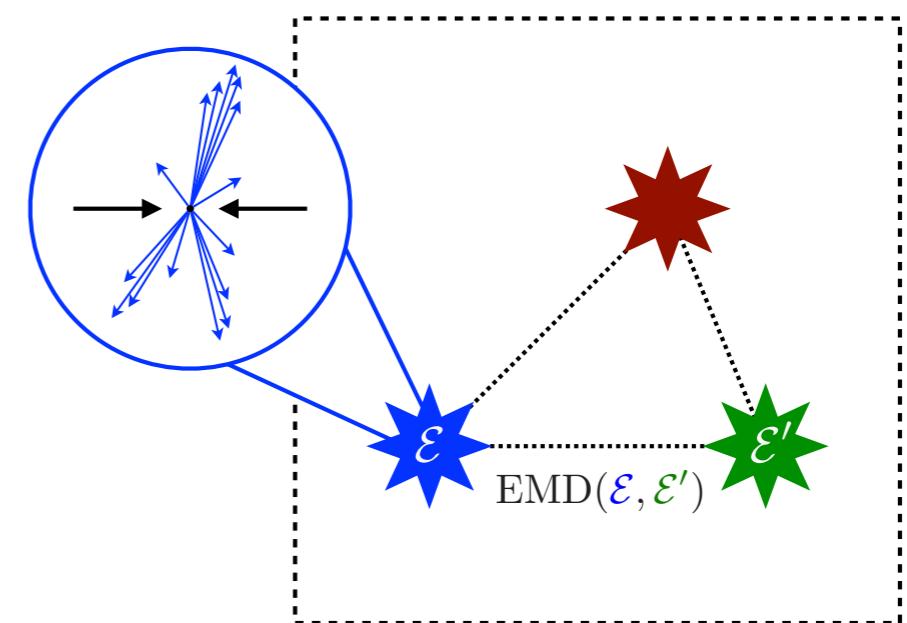
[Komiske, Mastandrea, Metodiev, Naik, JDT, [PRD 2020](#);
using van der Maaten, Hinton, [JMLR 2008](#); using [CMS Open Data](#)]



Building the Forest from the Trees



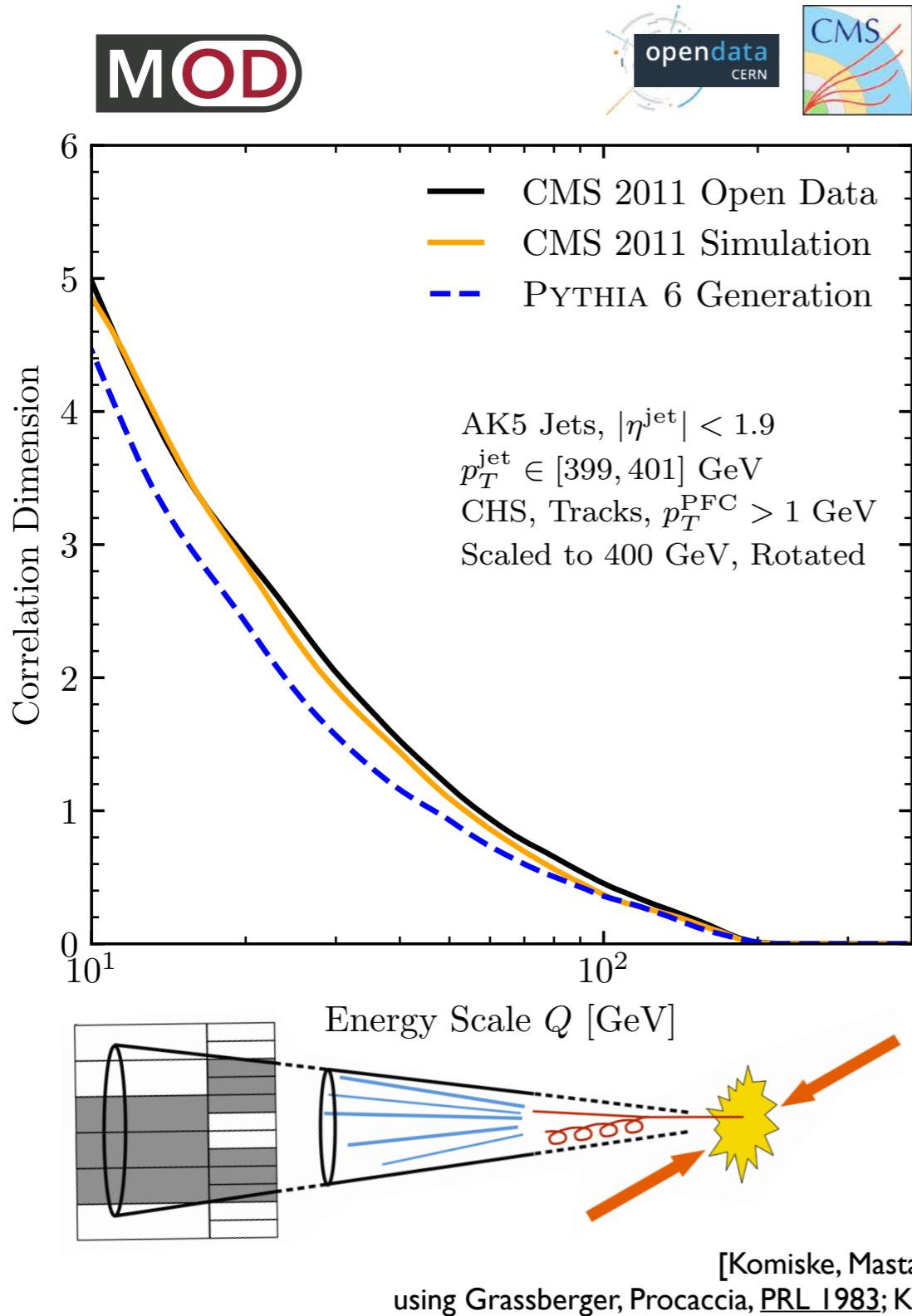
The Space of Energy Flows



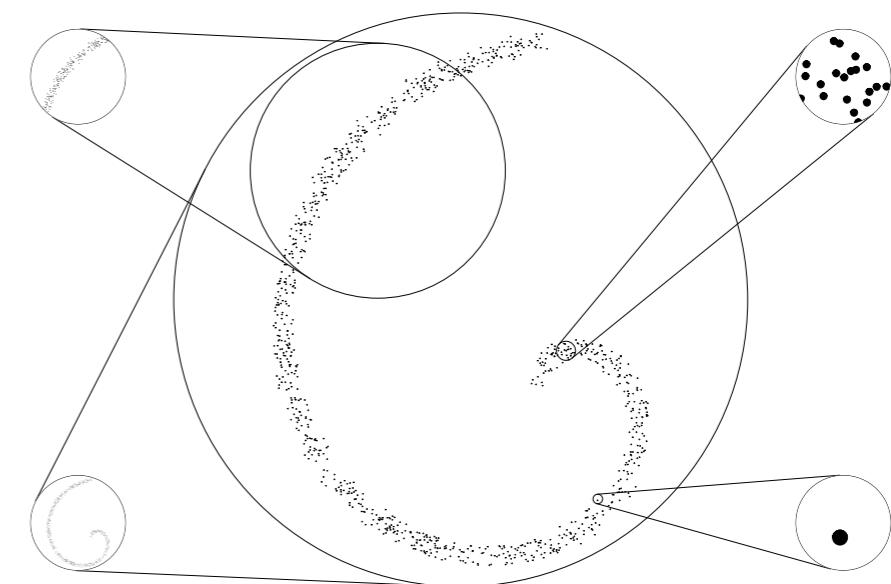
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;
using van der Maaten, Hinton, JMLR 2008; using CMS Open Data]

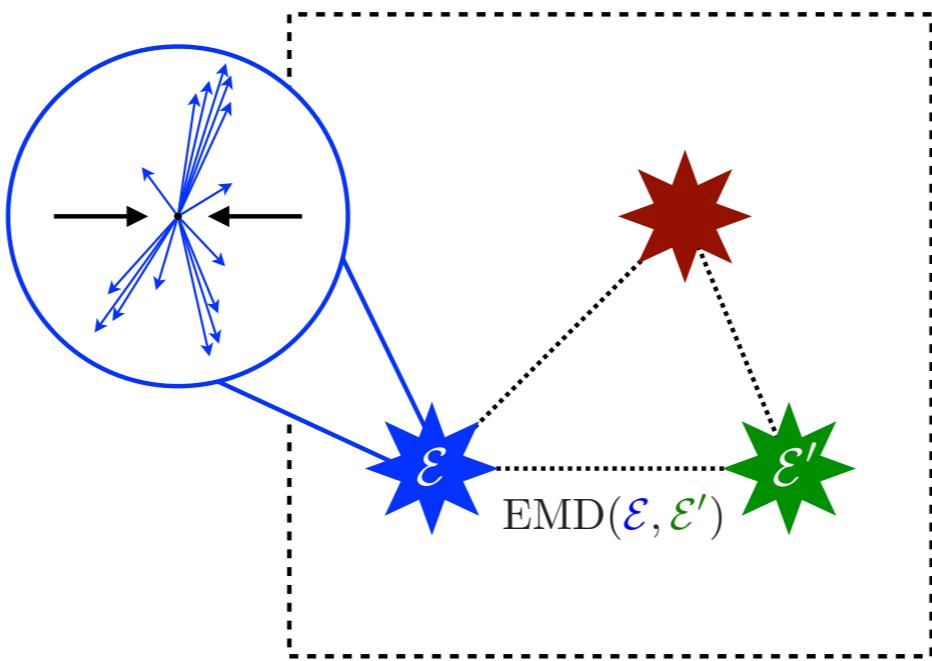


A Super-Fractal Forest made from Trees

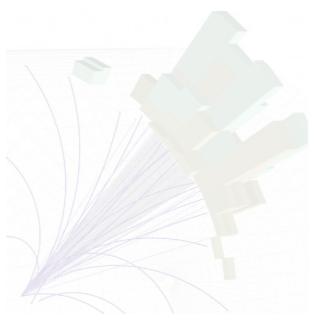


Dimension of Space of Energy Flows

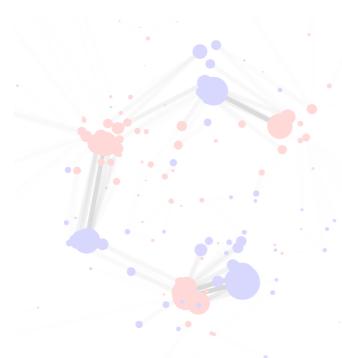




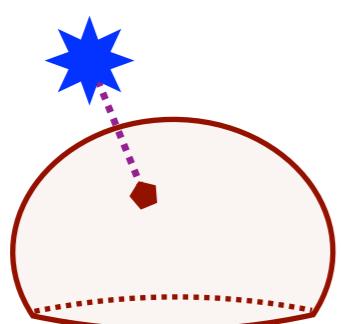
*Viewed through the data science lens,
the EMD unlocks a suite of
geometric analysis strategies*



Going with the (Energy) Flow



The Energy Mover's Distance

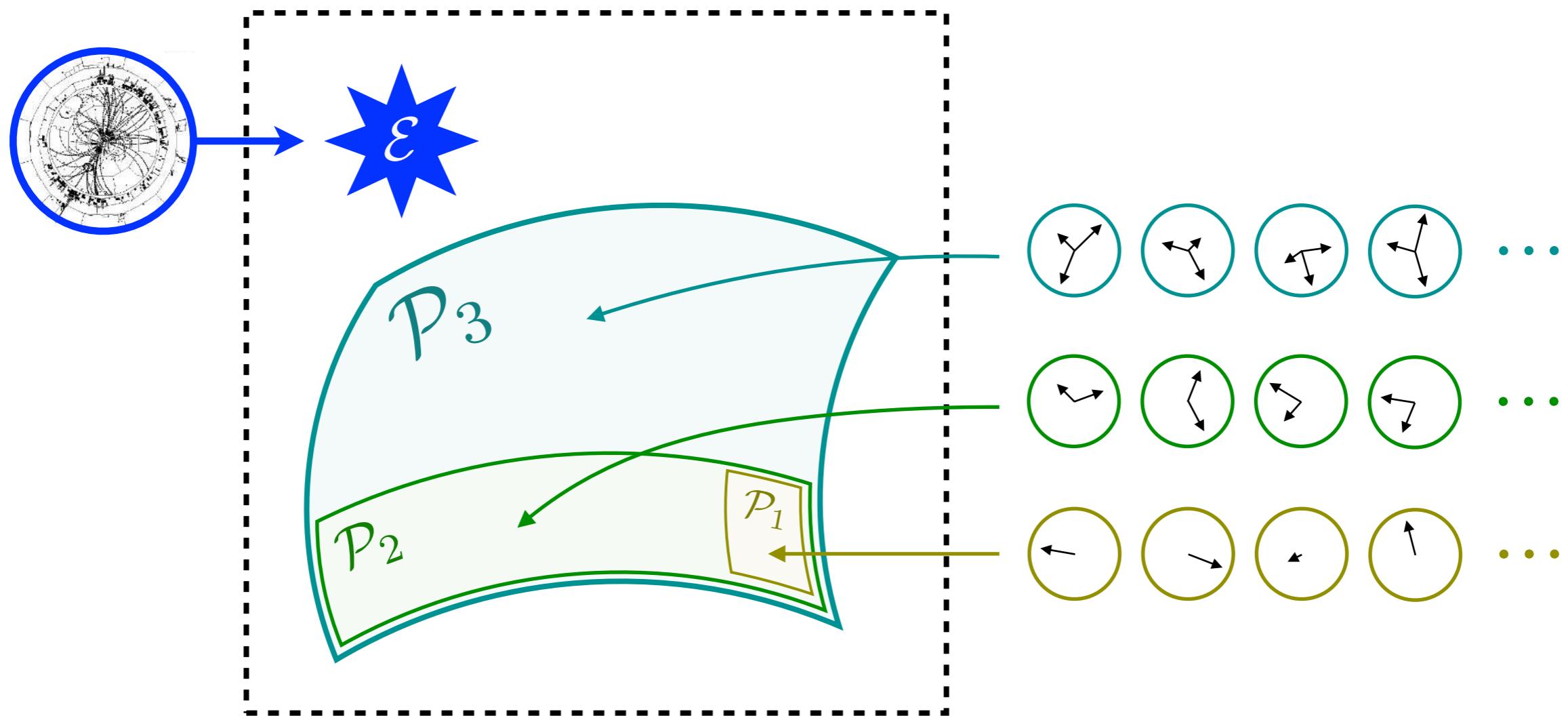


Revealing a Hidden Geometry

*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

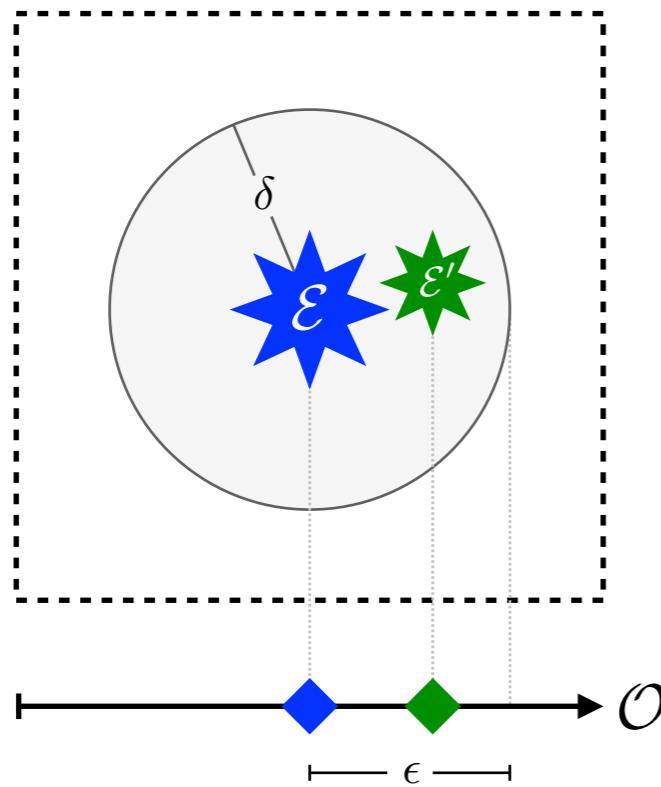


$\mathcal{P}_N \supset \mathcal{P}_{N-1} \supset \dots \supset \mathcal{P}_2 \supset \mathcal{P}_1$ by soft/collinear limits

[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]

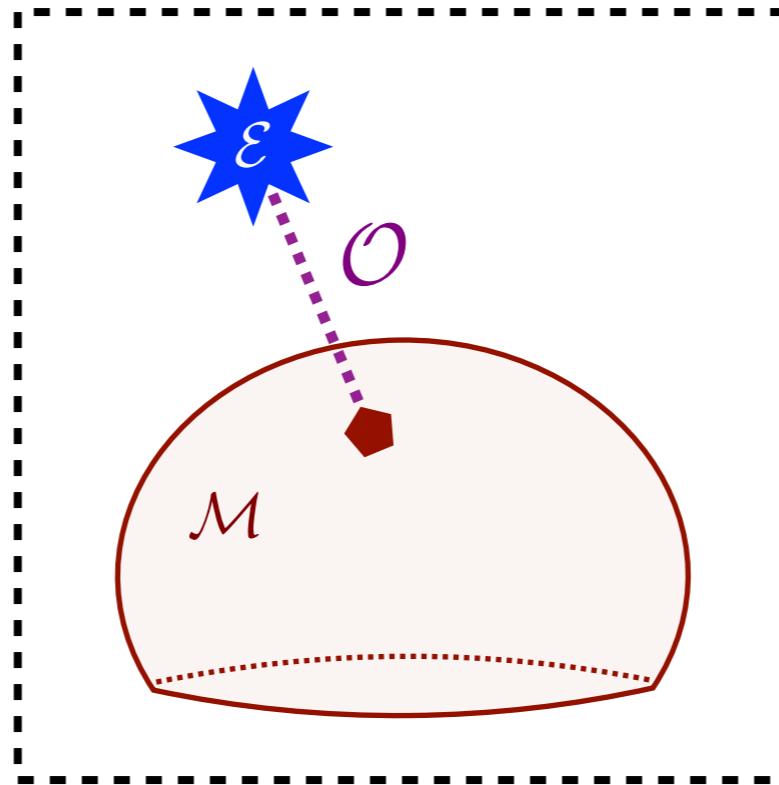
[see also Banfi, Salam, Zanderighi, JHEP 2005; Larkoski, Marzani, JDT, PRD 2015]

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

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

Manifolds for Observables

One Event



Set of Events

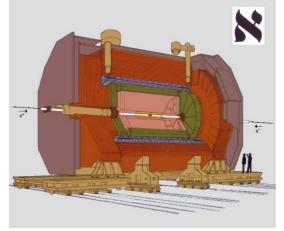
Distance of Closest Approach \Rightarrow Observable

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

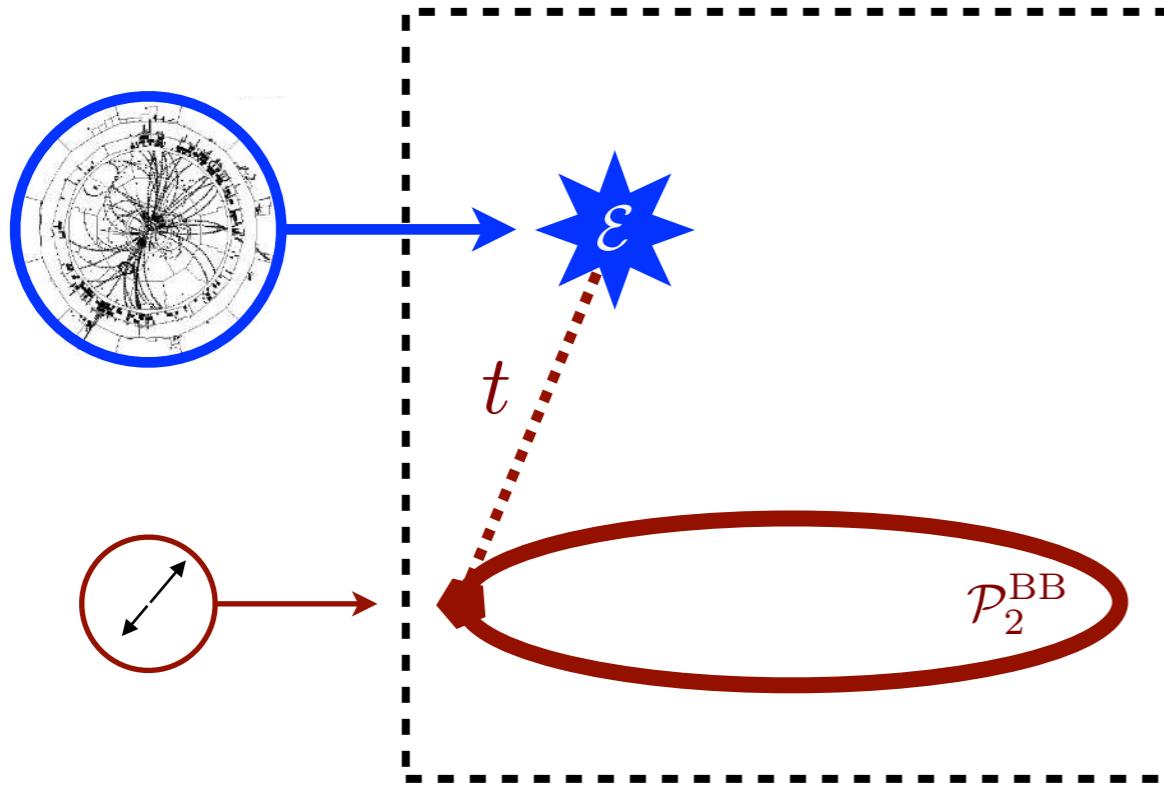
[Komiske, Metodiev, JDT, [JHEP 2020](#)]

E.g. Thrust

How dijet-like is an event?



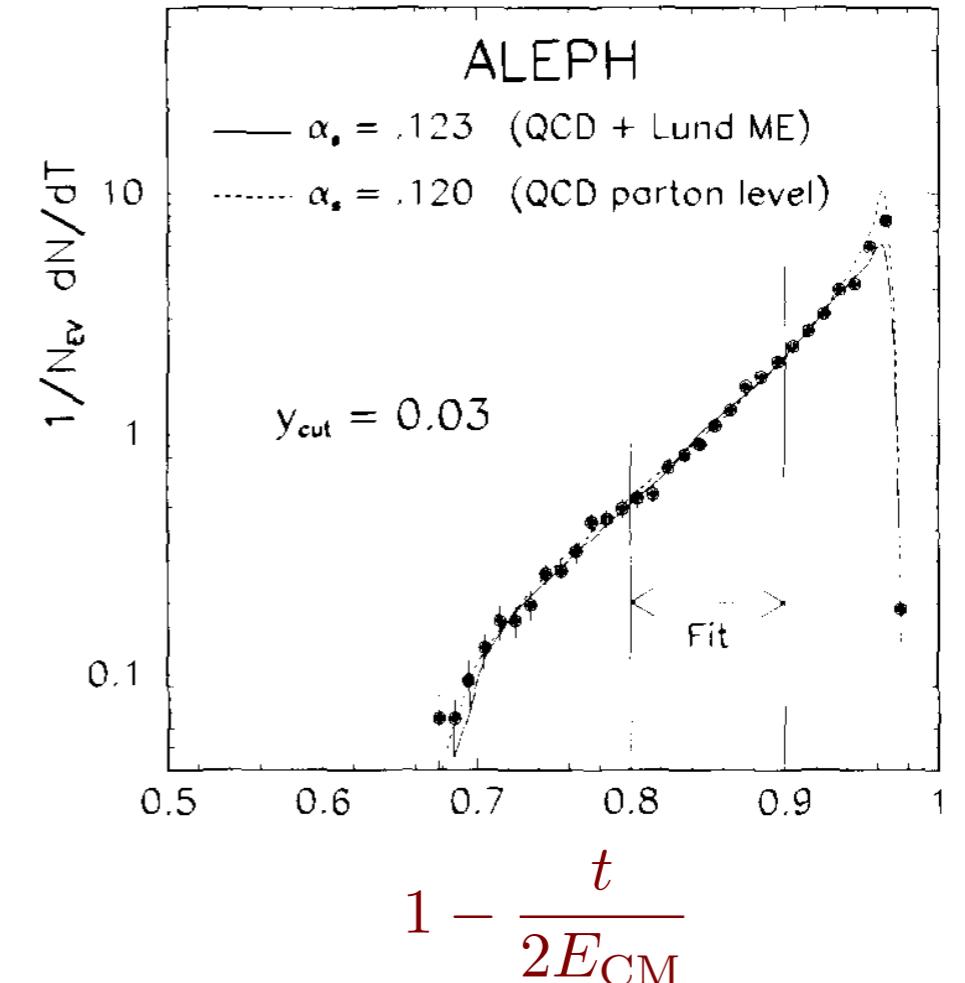
$$t(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{P}_2^{\text{BB}}} \text{EMD}_2(\mathcal{E}, \mathcal{E}')$$



All Back-to-Back Two Particle Configurations

$$\mathcal{P}_2^{\text{BB}} = \left\{ \begin{array}{c} \text{red circles with two arrows pointing away from each other} \\ \dots \end{array} \right\}$$

(using $\beta=2$ EMD variant)



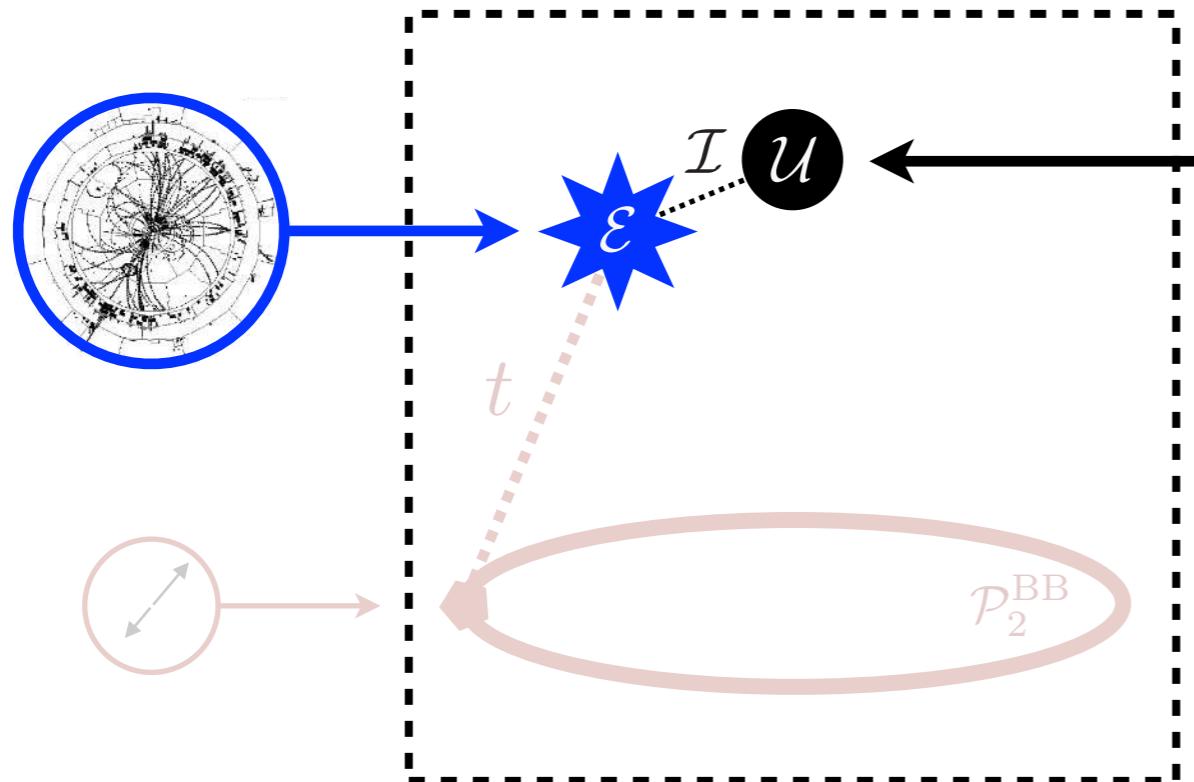
$$1 - \frac{t}{2E_{\text{CM}}}$$

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

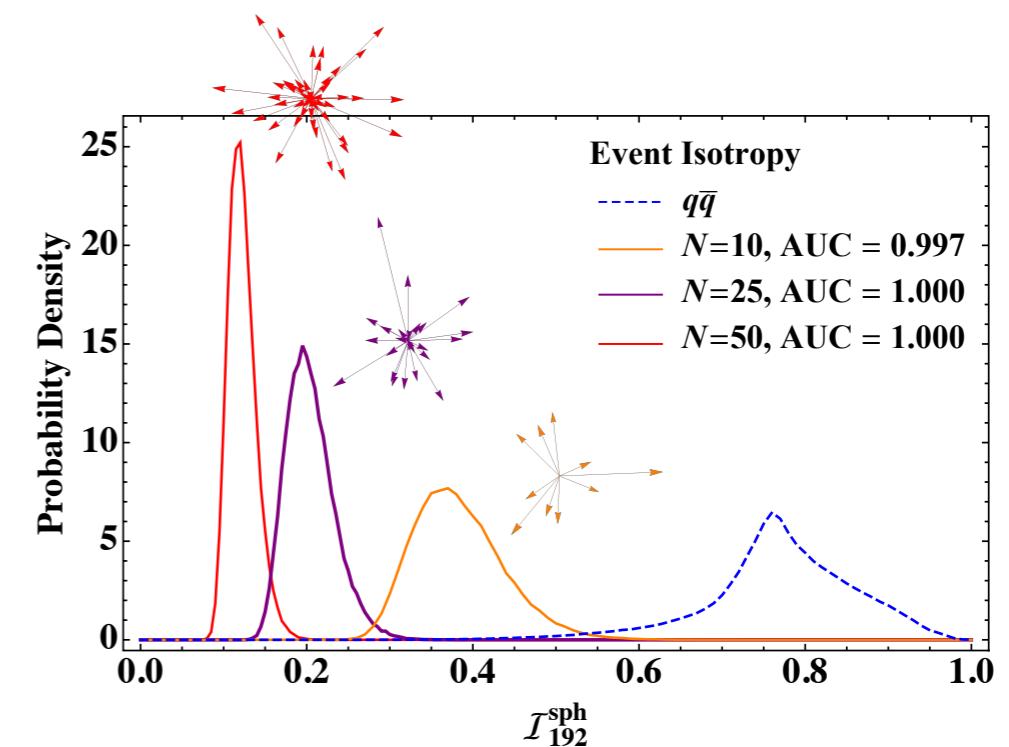
[Komiske, Metodiev, JDT, JHEP 2020]
 [Brandt, Peyrou, Sosnowski, Wroblewski, PL 1964; Farhi, PRL 1977; ALEPH, PLB 1991]

New! Event Isotropy

How isotropic is an event?



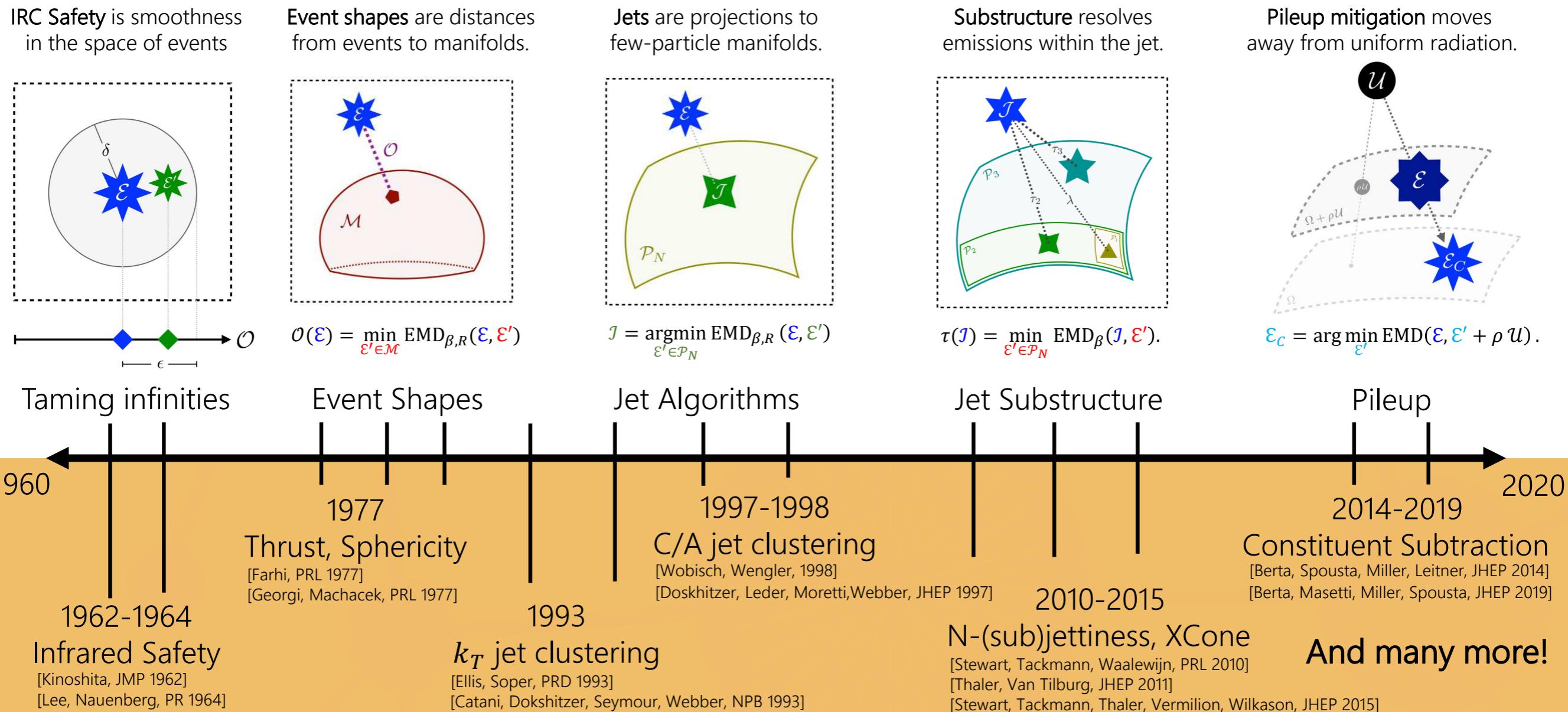
$$\mathcal{I}(\mathcal{E}) = \text{EMD}(\mathcal{E}, \mathcal{U})$$



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



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

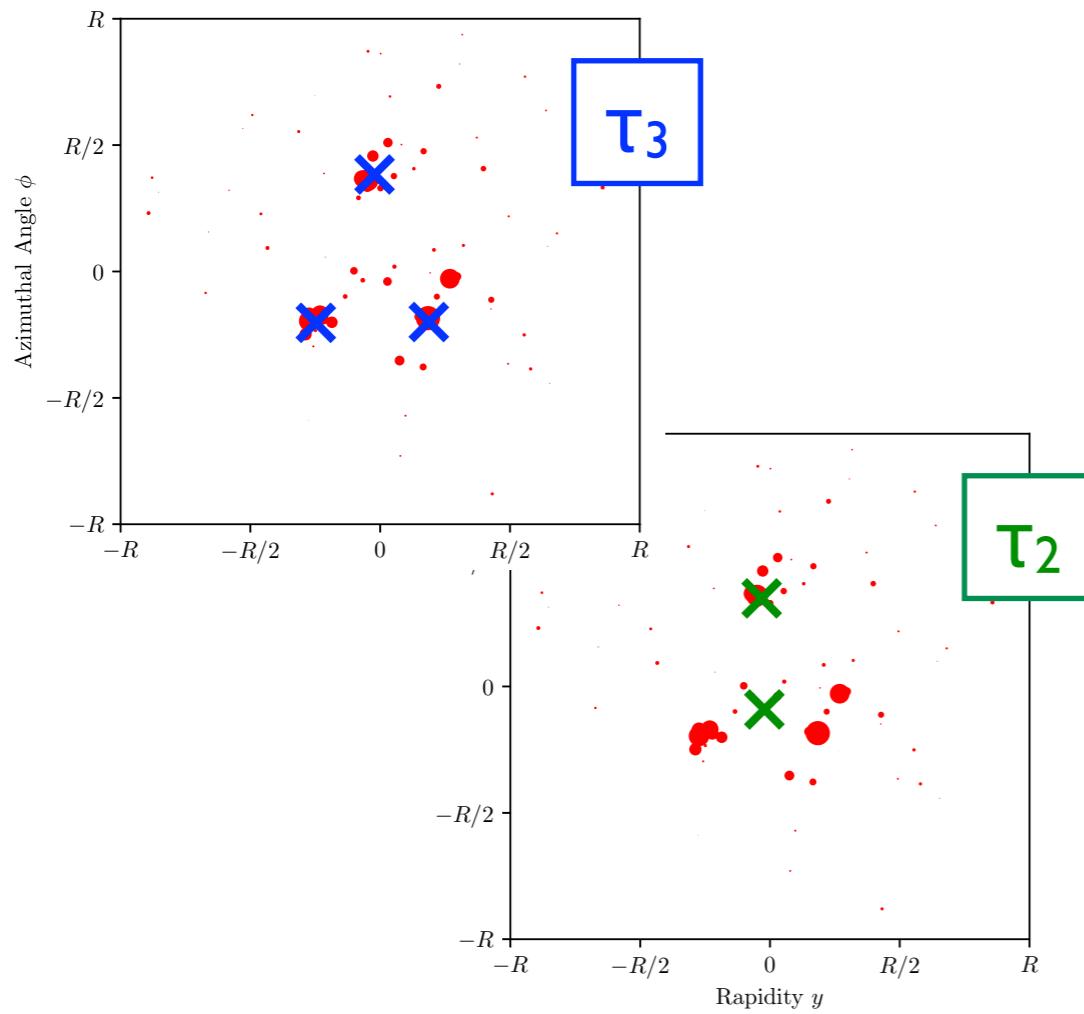


[Komiske, Metodiev, JDT, JHEP 2020; timeline from Metodiev]

N-subjettiness

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

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



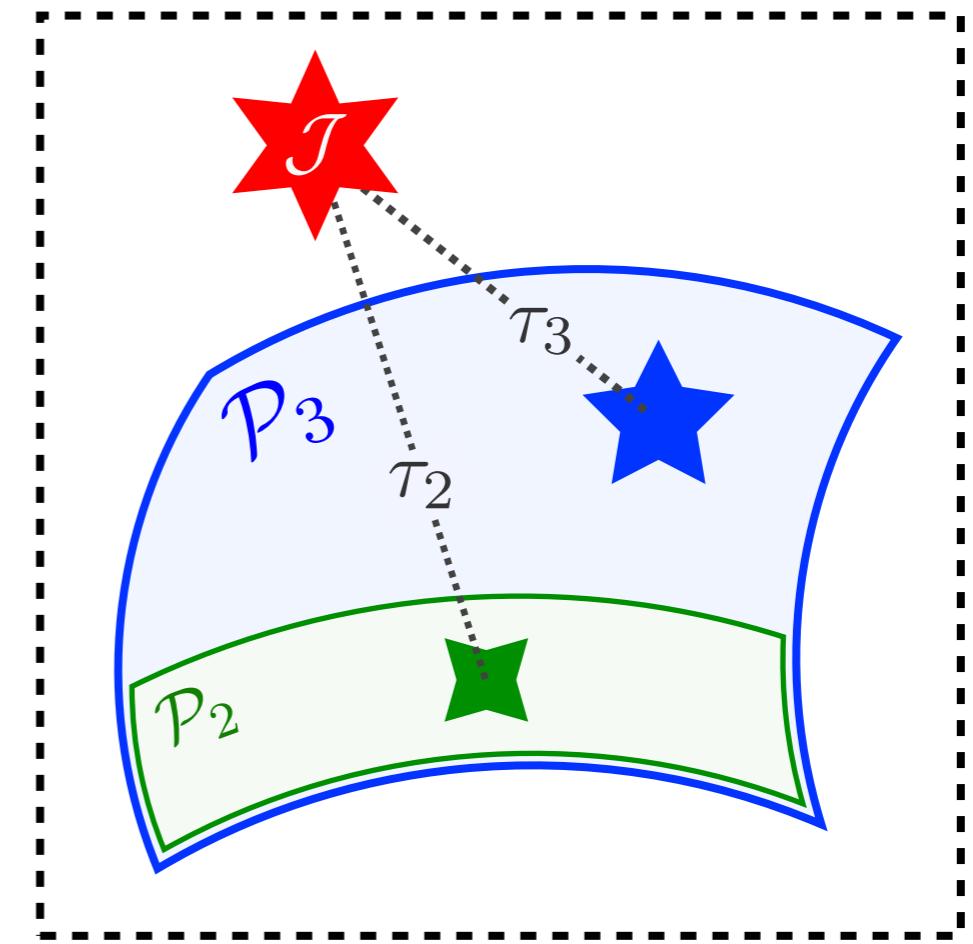
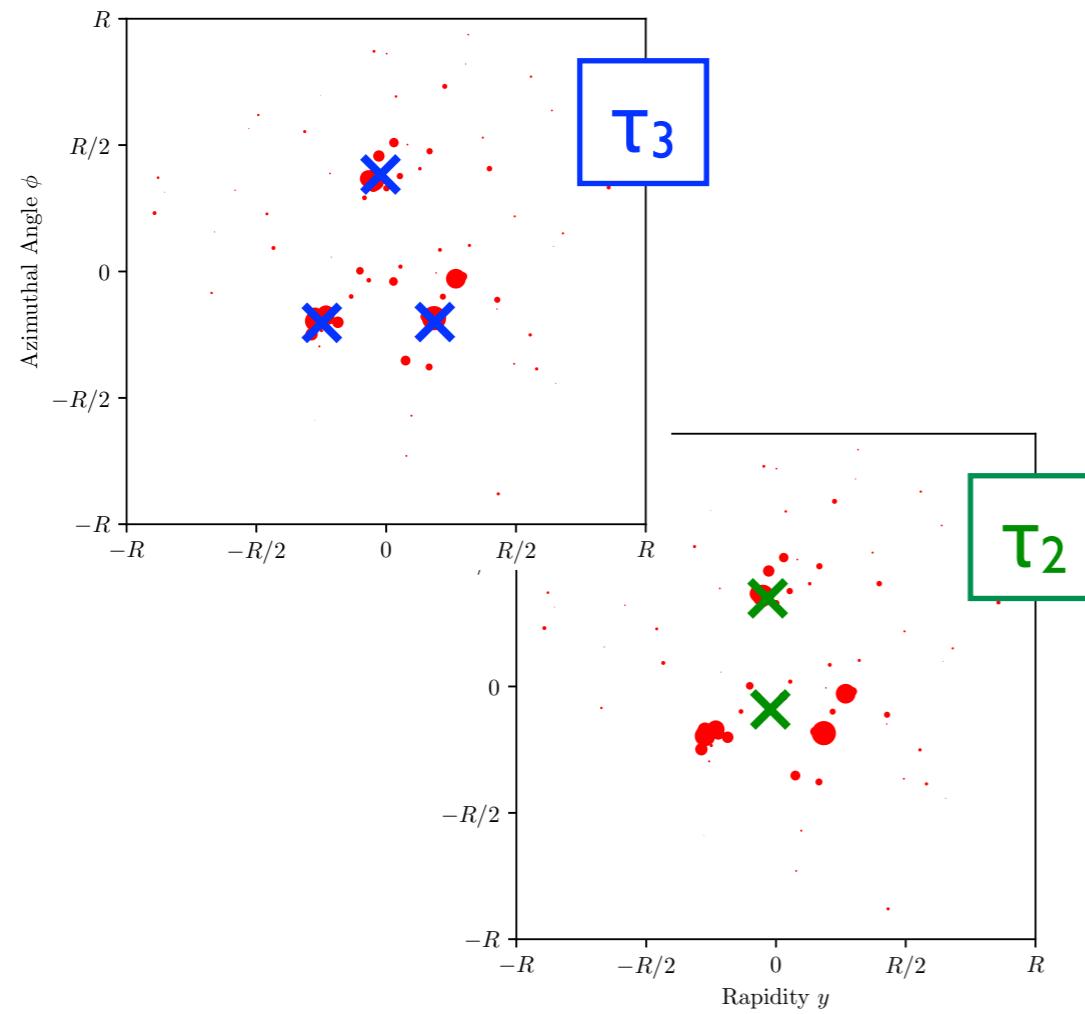
[JDT, Van Tilburg, [JHEP 2011](#), [JHEP 2012](#);
based on Brandt, Dahmen, [ZPC 1979](#); Stewart, Tackmann, Waalewijn, [PRL 2010](#)]



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]

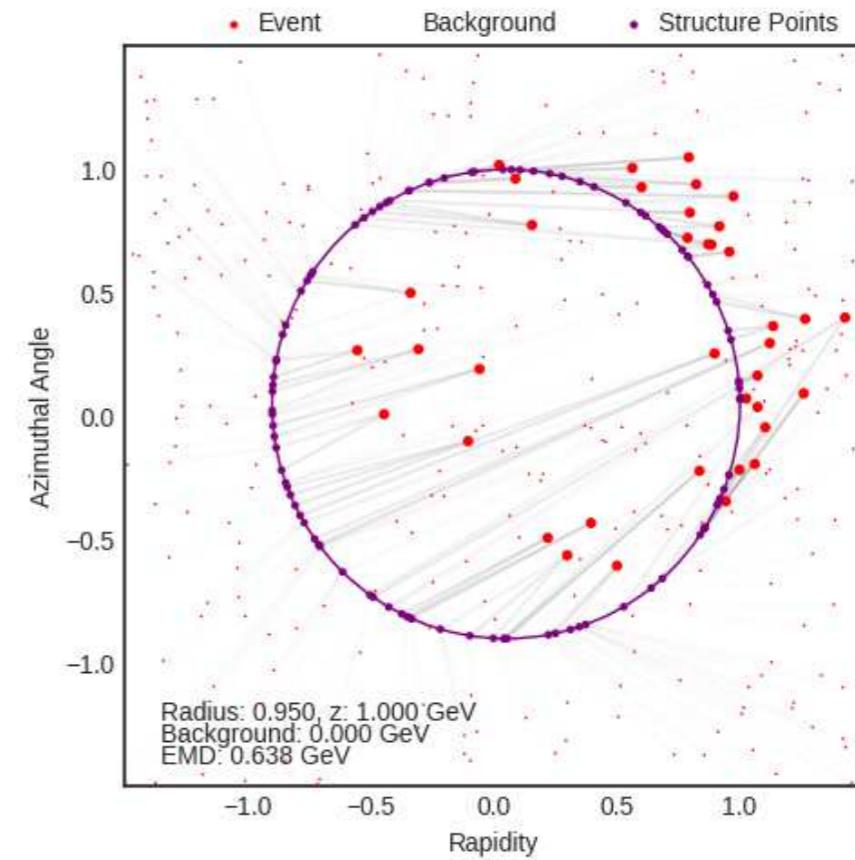
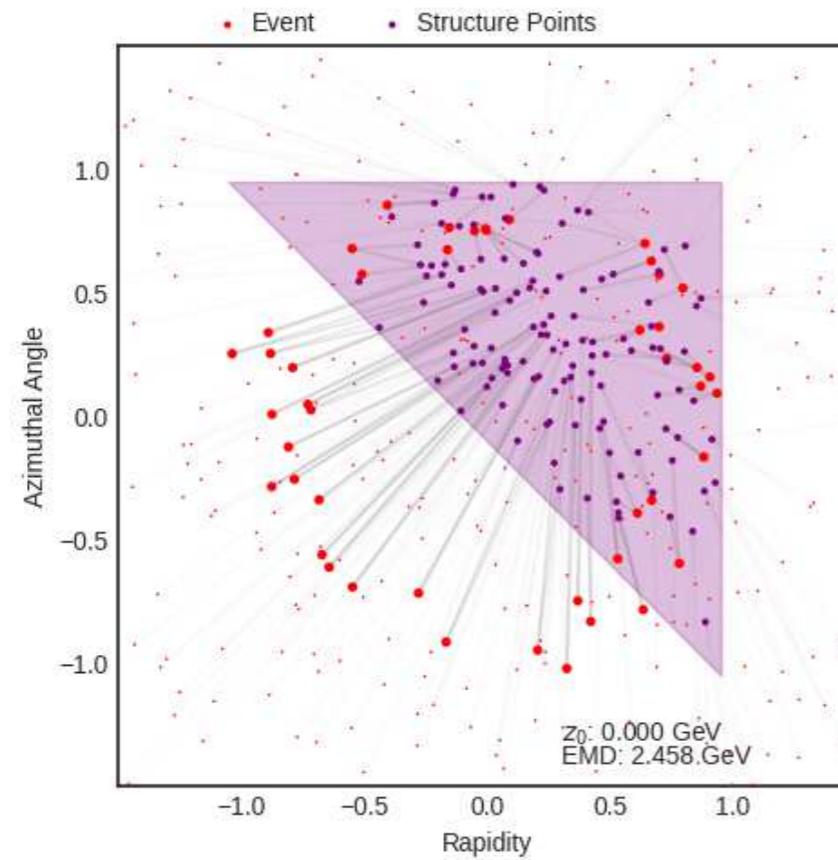


Deep Manifold Learning

Optimal transport meets gradient descent

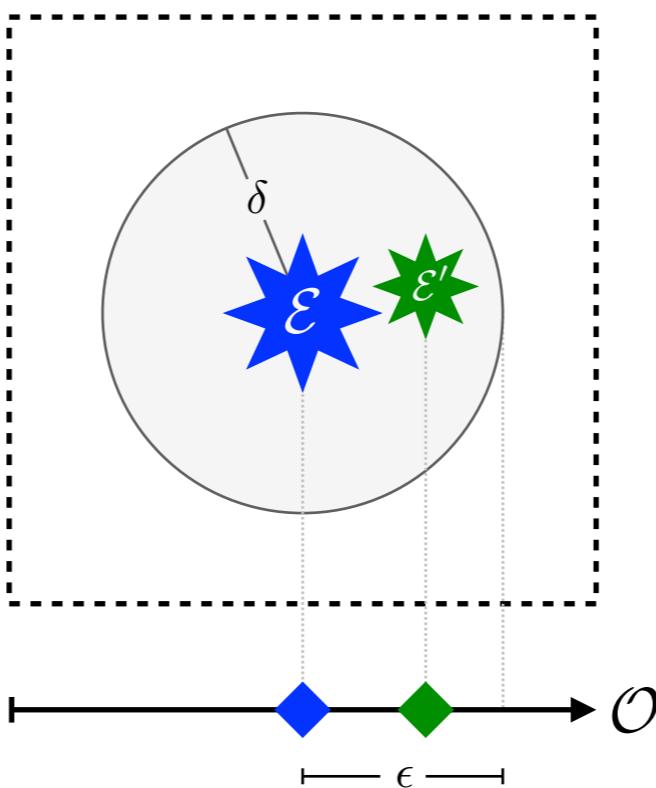
$$\mathcal{O}(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{M}} \text{EMD}(\mathcal{E}, \mathcal{E}')$$

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



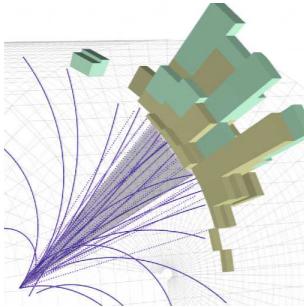
[Ba, Dogra, Gambhir, JDT, in progress;
inspired by Tankala, Tasissa, Murphy, Ba, [arXiv 2020](#)]





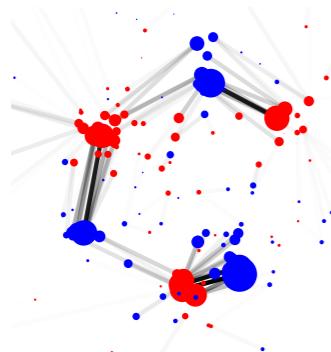
*We are just beginning to leverage the
conceptual richness of optimal transport
for high-energy physics application*

Summary



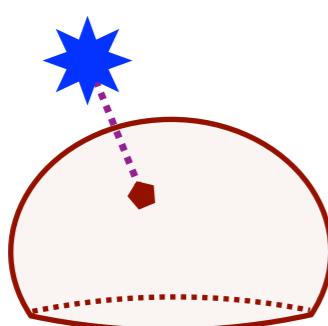
Going with the (Energy) Flow

*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*

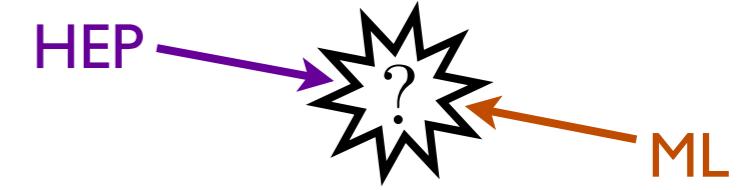


Revealing a Hidden Geometry

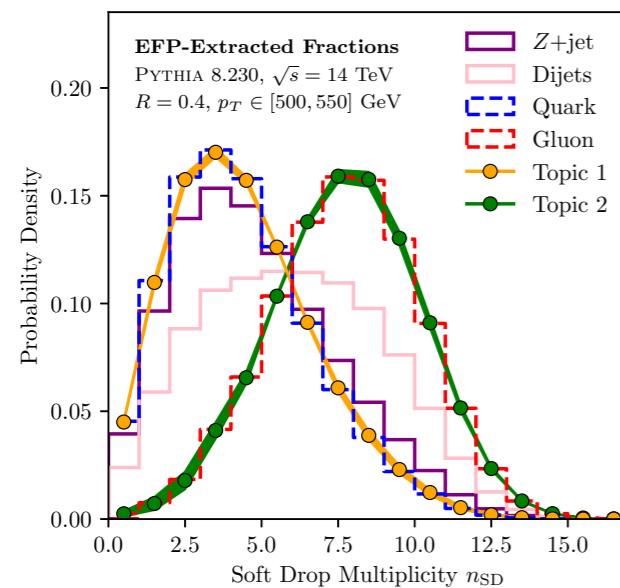
*We can gain new perspectives on concepts/techniques
in QFT and collider physics from the last half century*

Backup Slides

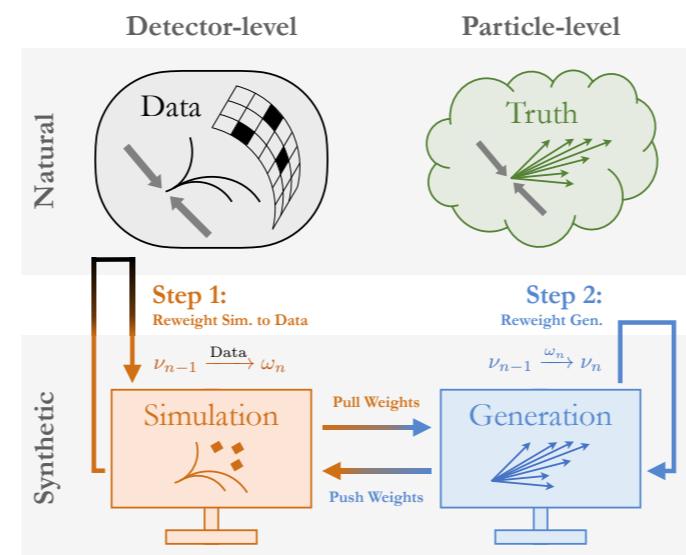
Recent Collisions



Quark/Gluon Definitions via Blind Source Separation



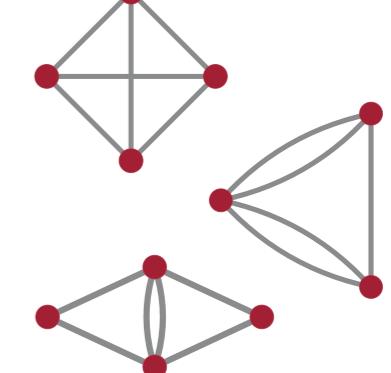
Detector Deconvolution via Binary Classification



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

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

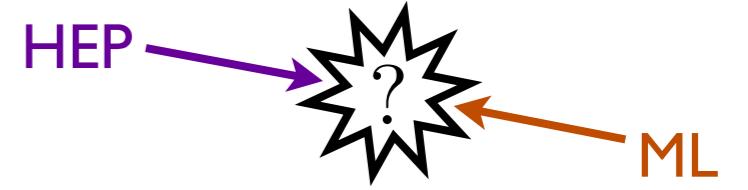


[Andreassen, Komiske, Metodiev,
Nachman, JDT, [PRL 2020](#)]

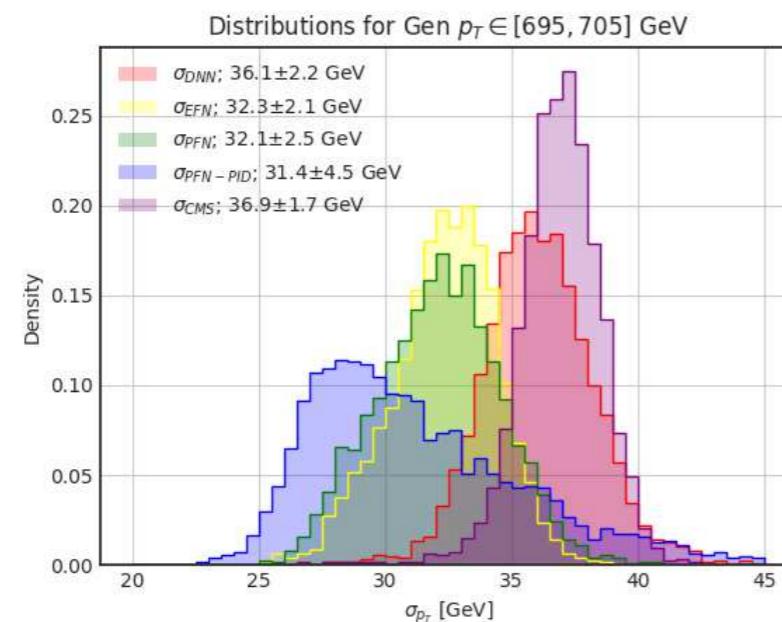
[Komiske, Metodiev, JDT,
[JHEP 2018](#), [PRD 2020](#)]

High Energy Physics \leftrightarrow Mathematics, Statistics & Computer Science

Ongoing Collisions

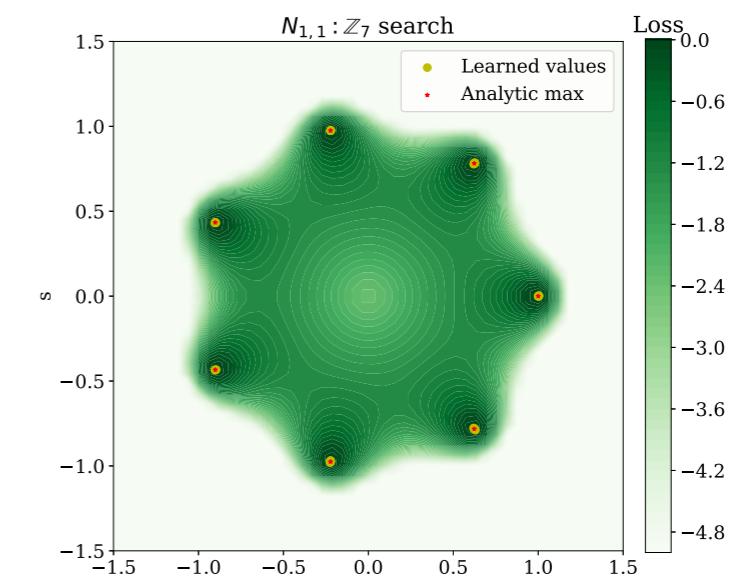


Frequentist Jet Calibration via Gaussian Ansatz



[Nachman, Gambhir, JDT, in progress]

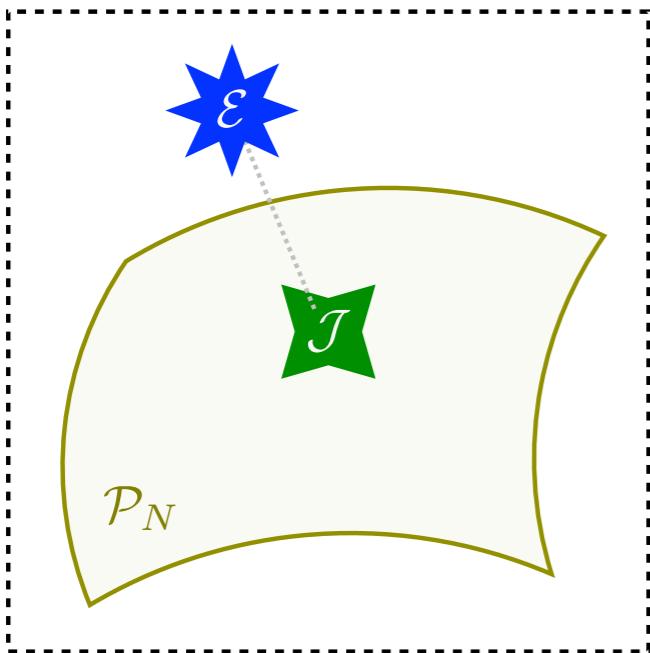
Symmetry Discovery via Adversarial Learning



[Desai, Nachman, JDT, NeurIPS 2021 ML4PS]

High Energy Physics \leftrightarrow Mathematics, Statistics & Computer Science

More Fun with N-particle Manifolds



N-jettiness

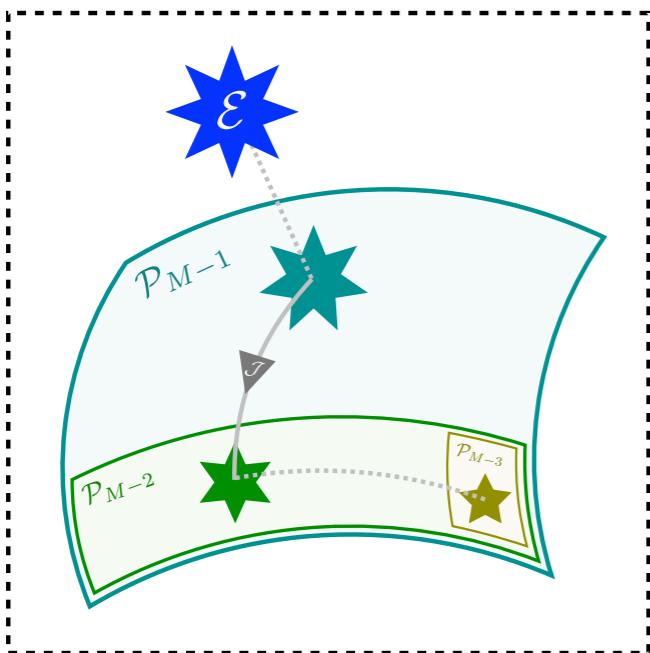
Distance of closest approach to N-particle manifold

[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

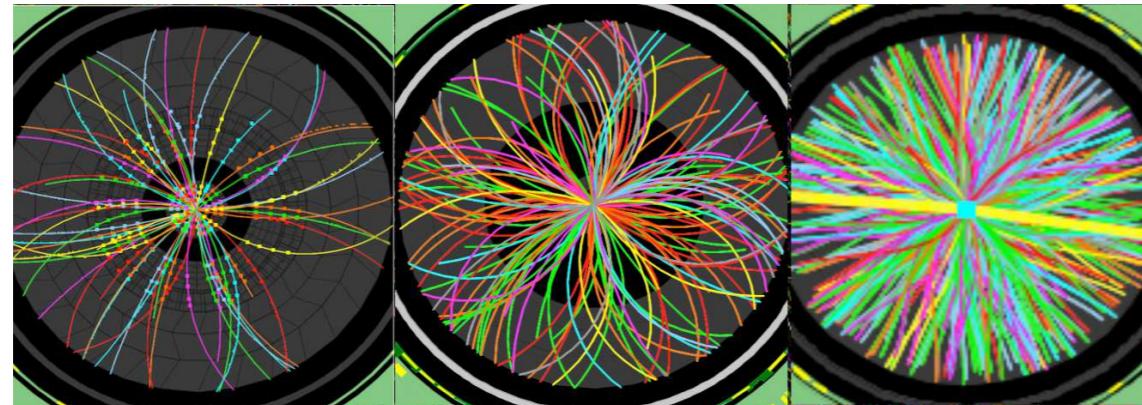
[Catani, Dokshitzer, Seymour, Webber, [NPB 1993](#); Ellis, Soper, [PRD 1993](#)]

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

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

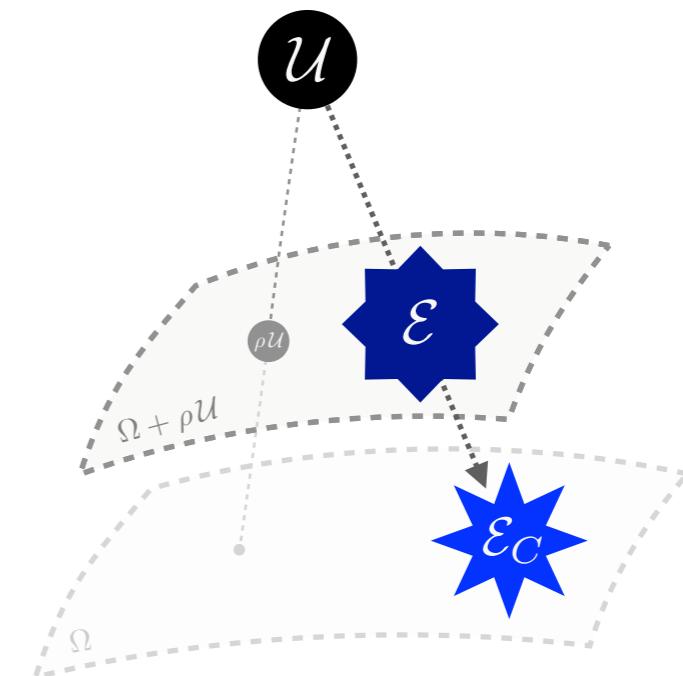
[Komiske, Metodiev, JDT, [JHEP 2020](#)]

Pileup Mitigation



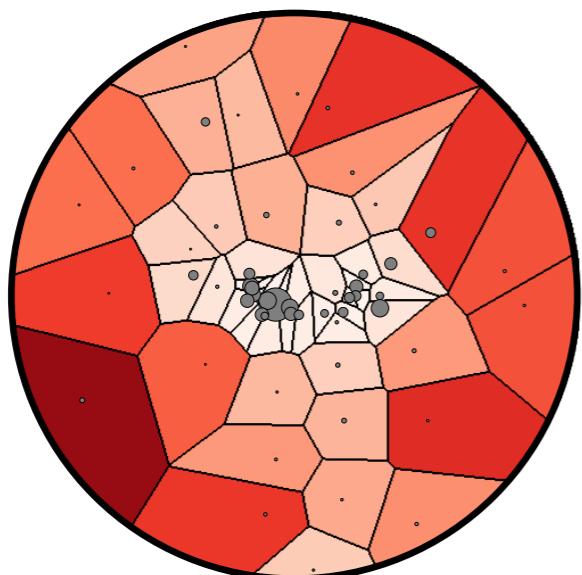
[see review in Soyez, PR 2019]

Uniform event contamination from overlapping proton-proton collisions



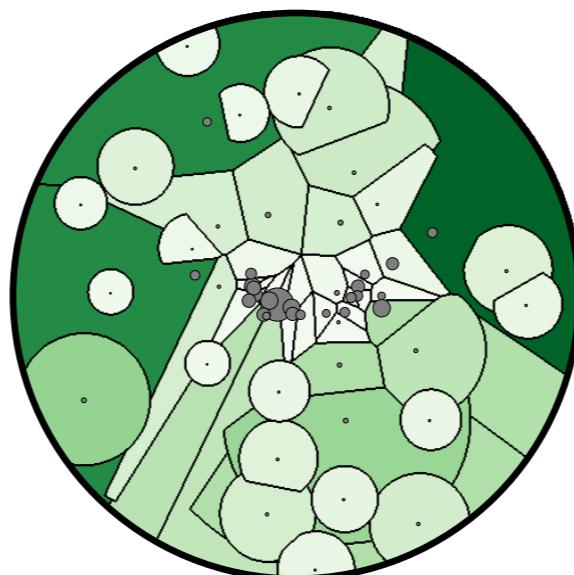
Pileup Mitigation:
“Move away” from uniform event

Voronoi



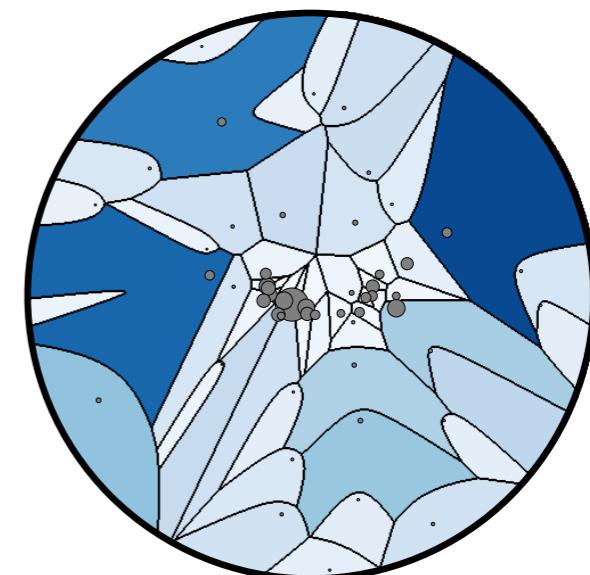
[Cacciari, Salam, Soyez, JHEP 2008]

Constituent Subtraction



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

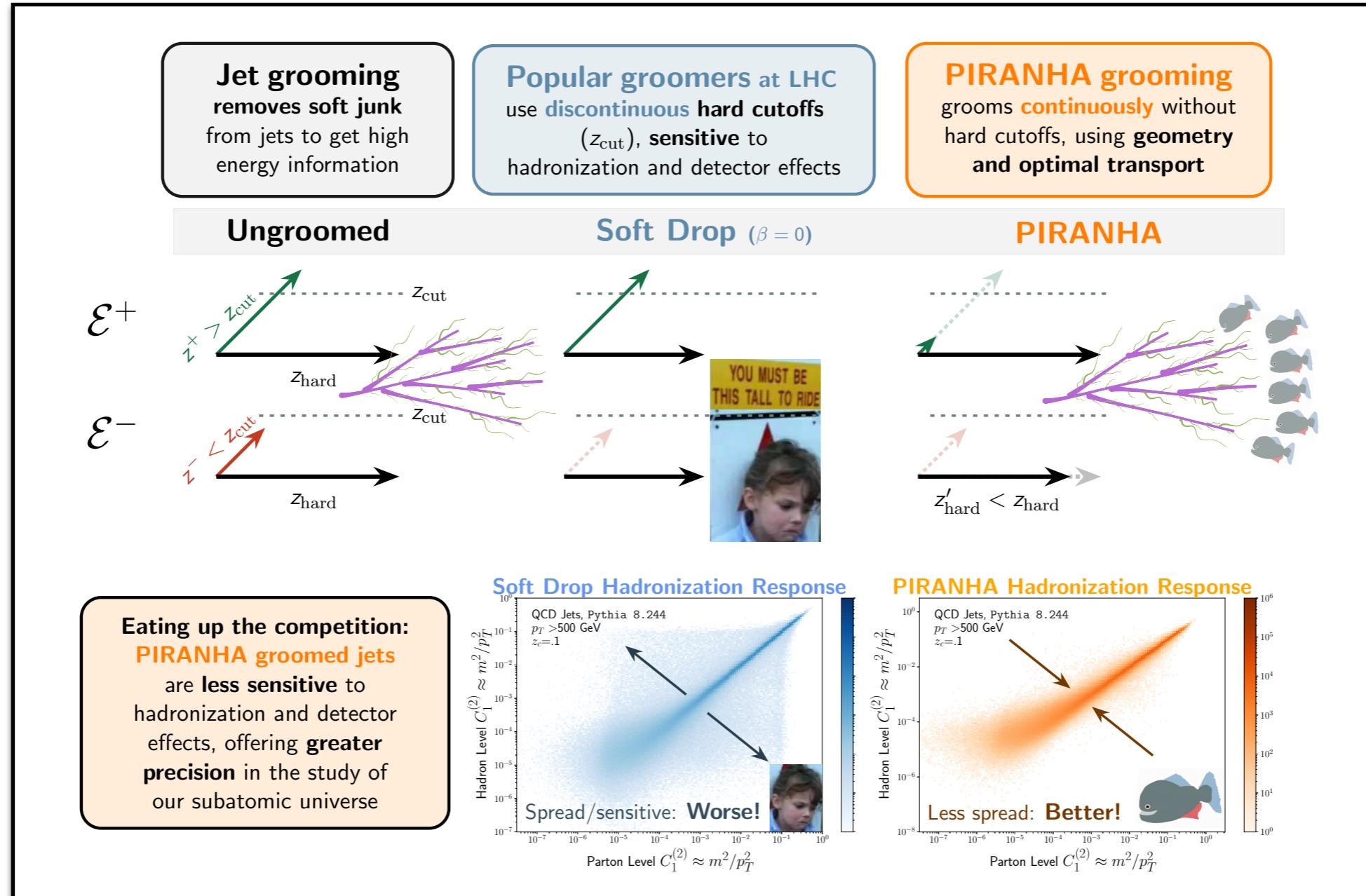
Apollonius



[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]

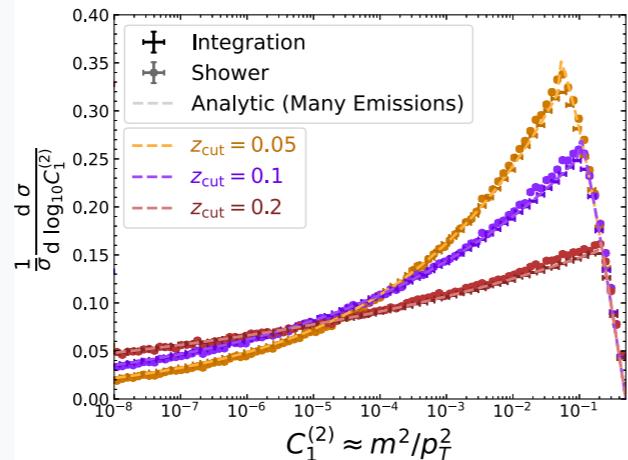


Pileup and Infrared Radiation AnNiHilAtion

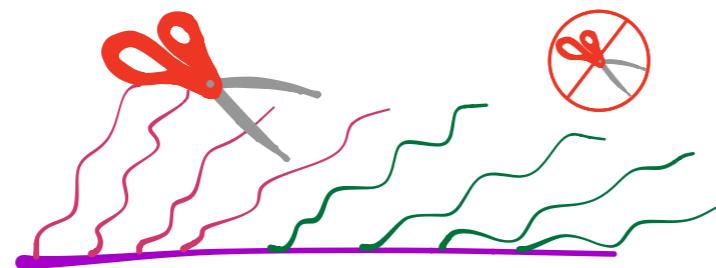
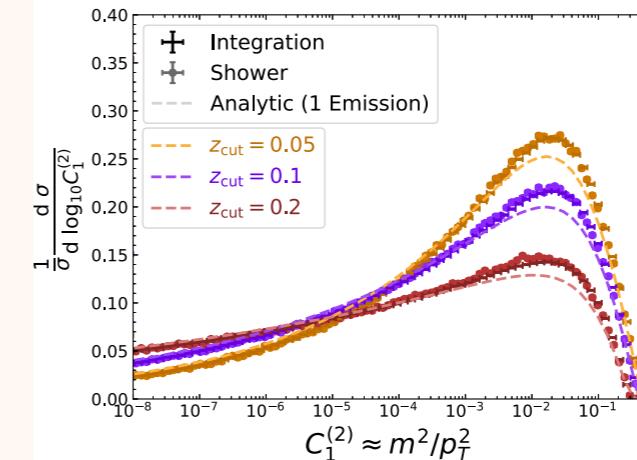
Recursive Safe Subtraction: tree-based approx. to optimal transport grooming

Fixed coupling, **multiple emission** calculations:

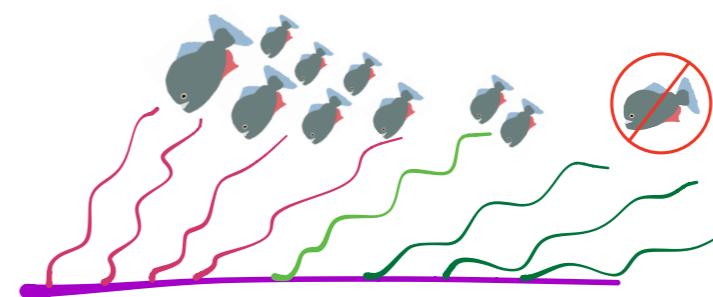
Soft Drop/mMDT



PIRANHA-RSS ($f = 1$)



Sharp cutoff → kink



No sharp cutoff → smooth

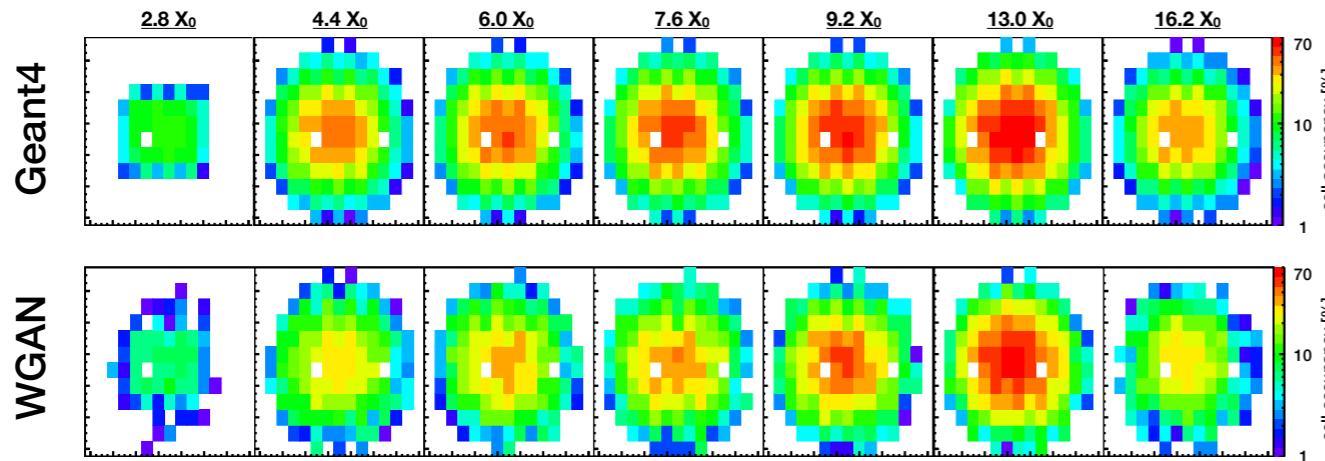
[Slides from Sam Alipour-fard]

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



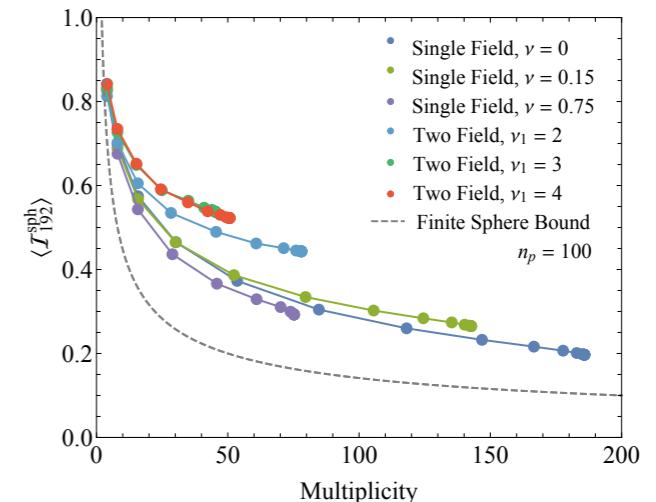
Wasserstein in HEP

Generative Modeling



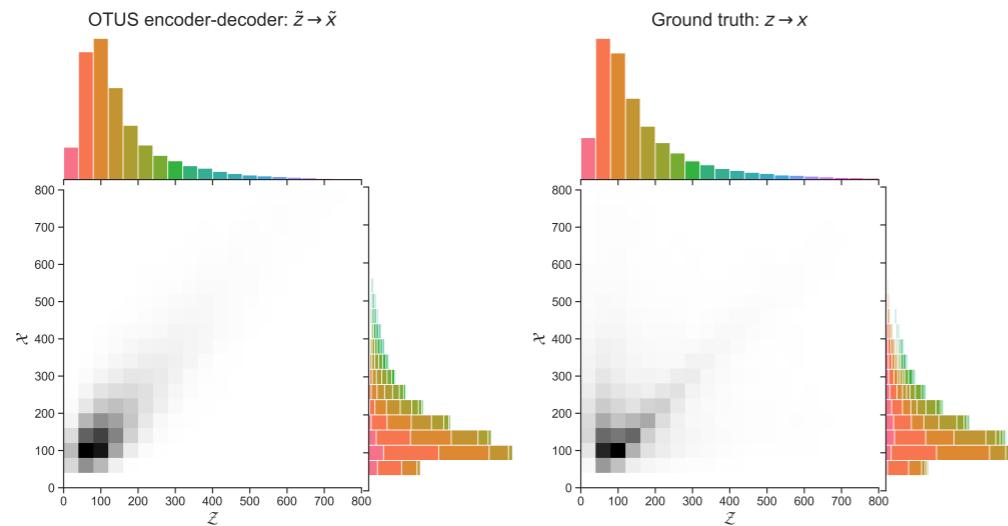
[Erdmann, Geiger, Glombitza, Schmidt, [CSBS 2018](#); Erdmann, Glombitza, Quast, [CSBS 2019](#);
Chekalina, Orlova, Ratnikov, Ulyanov, Ustyuzhanin, Zakharov, [CHEP 2018](#)]

BSM Characterization



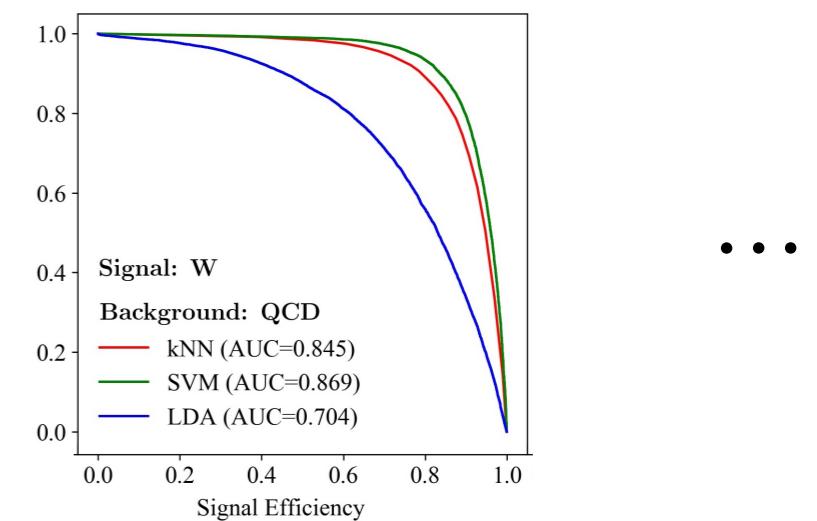
[Cesarotti, Reece, Strassler, [JHEP 2021](#), [arXiv 2020](#)]

Estimated Simulation/Unfolding



[Howard, Mandt, Whiteson, Yang, [arXiv 2021](#)]

Jet Classification



[Cai, Cheng, Craig, Craig, [PRD 2020](#)]