

Optimal Transport for QCD and Jets

Jesse Thaler

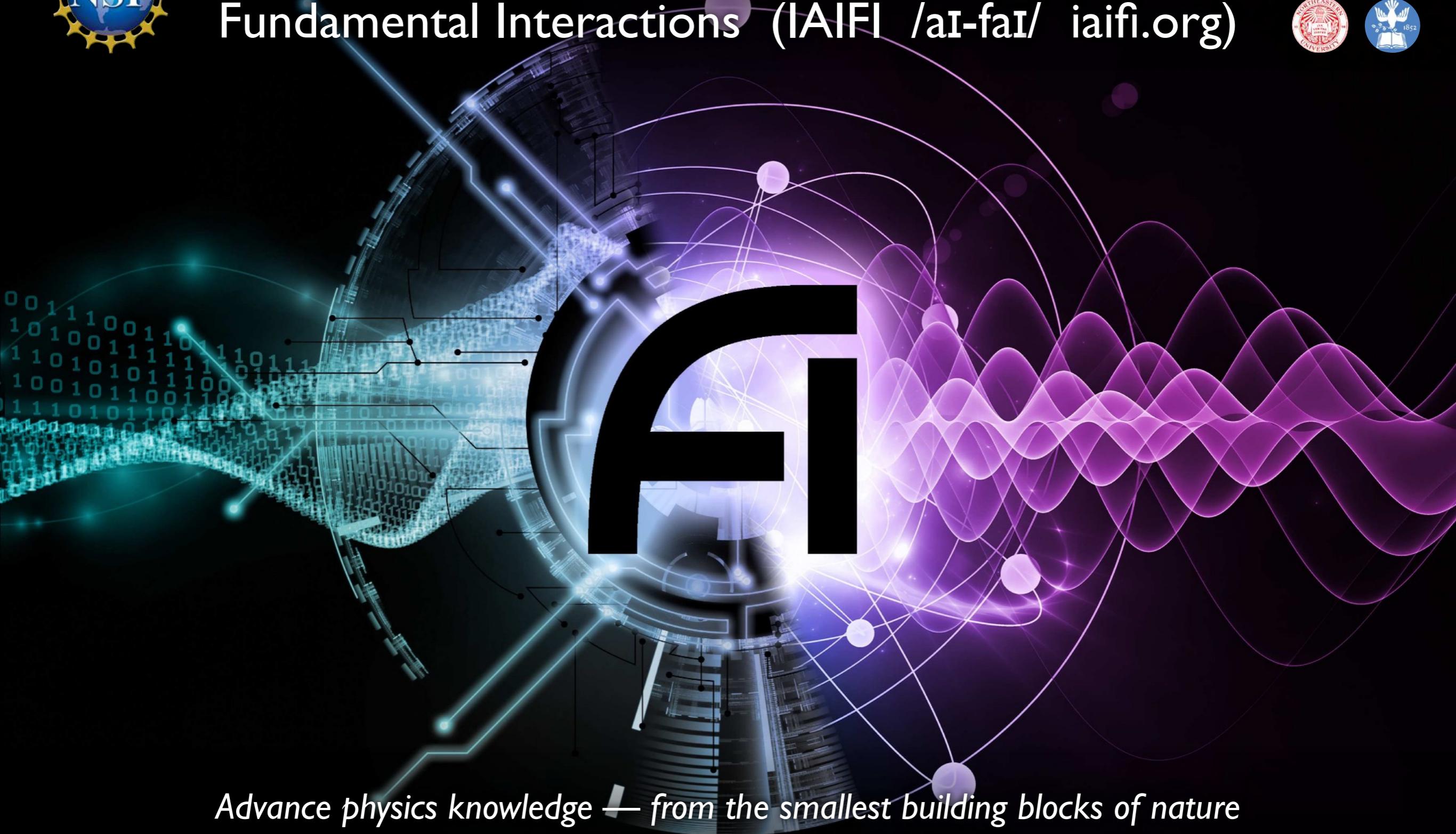


21

Flowing into the Future, Simons Center for Geometry and Physics — March 22, 2022



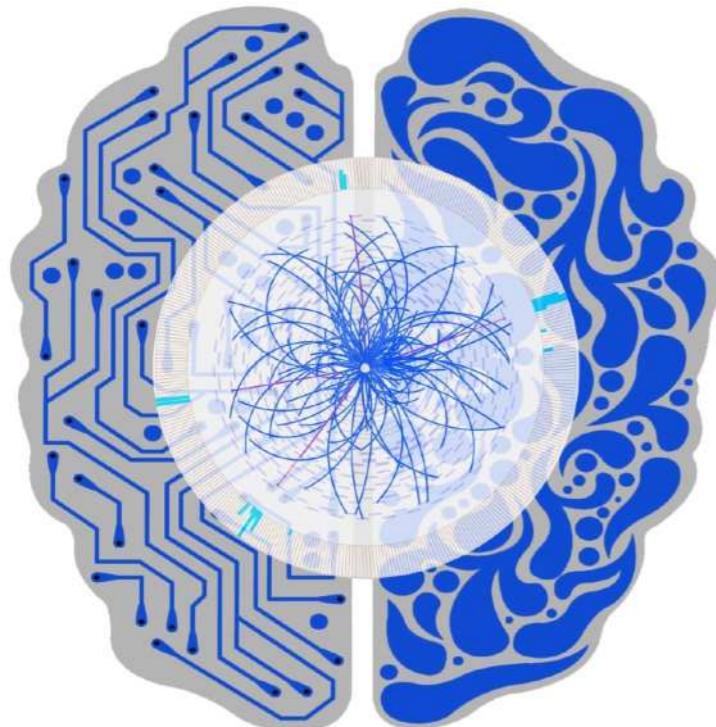
The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI /aI-faI/ iaifi.org)



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



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



*Infuse physics intelligence
into artificial intelligence*

Symmetries, conservation laws, scaling relations, limiting behaviors, locality, causality, unitarity, gauge invariance, entropy, least action, factorization, unit tests, exactness, systematic uncertainties, reproducibility, verifiability, ...

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

My QCD Wish List



- I) Understand **real-time dynamics** of hadronization
- 2) Build a **systematically improvable** parton shower
- 3) **Automate** perturbative calculations without subtractions
- 4) Rigorously define **theoretical uncertainties**

*Could machine learning / data science perspective
yield insights into any of these challenges?*

If you squint, optimal transport ideas are potentially relevant for each of these goals

Pushing the Frontiers of Collider Theory

$$\sigma_{\text{obs}} \simeq \frac{1}{2E_{\text{CM}}^2} \sum_{n=2}^{\infty} \int d\Phi_n |\mathcal{M}_{AB \rightarrow 12\dots n}|^2 f_{\text{obs}}(\Phi_n)$$

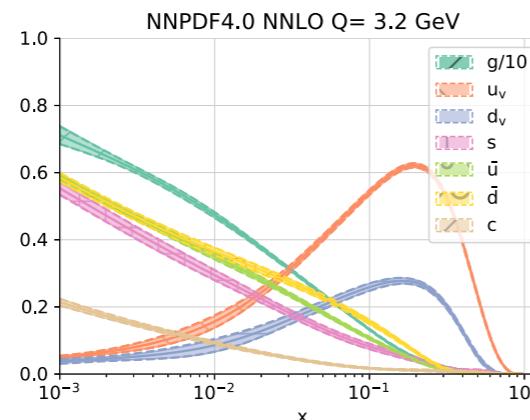
cross sectionphase spaceamplitudeobservable

Opportunity to rethink every ingredient in this formula

Pushing the Frontiers of Collider Theory

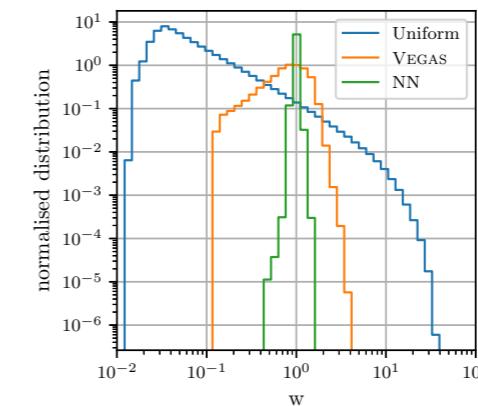
Machine Learning (Inspired) Advances

Parton Distribution Functions



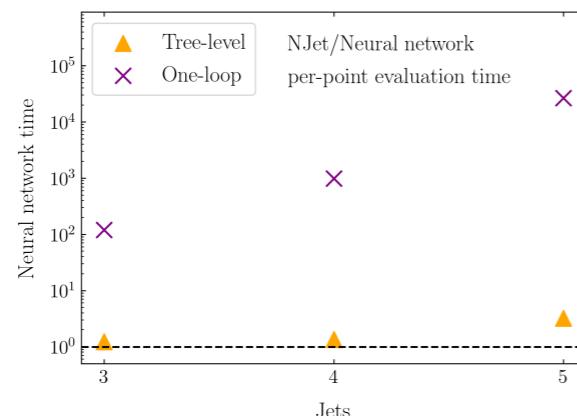
[e.g. NNPDF Collaboration, [JHEP 2022](#)]

Phase Space Integration



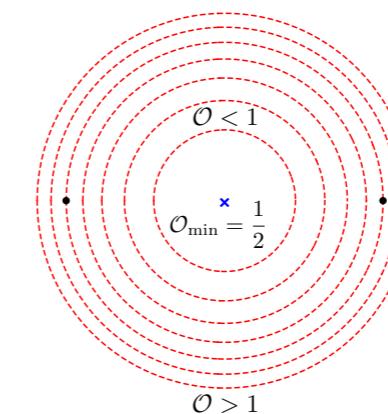
[e.g. Bothmann, Janßen, Knobbe, Schmale, Schumann, [SciPost 2020](#); see also Gao, Höche, Isaacson, Krause, Schulz, [PRD 2020](#)]

Amplitude Approximations



[e.g. Badger, Bullock, [JHEP 2020](#)]

Optimal Observables



[e.g. Buckley, Callea, Larkoski, Marzani, [SciPost 2020](#)]

Pushing the Frontiers of Collider Theory

$$\sigma_{\text{obs}} \simeq \frac{1}{2E_{\text{CM}}^2} \sum_{n=2}^{\infty} \int d\Phi_n |\mathcal{M}_{AB \rightarrow 12\dots n}|^2 f_{\text{obs}}(\Phi_n)$$

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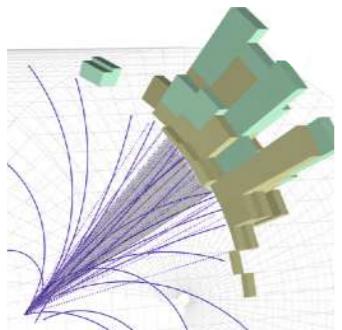
Opportunity to rethink every ingredient in this formula

*Opportunity to leverage new frameworks
to understand QCD and jets*

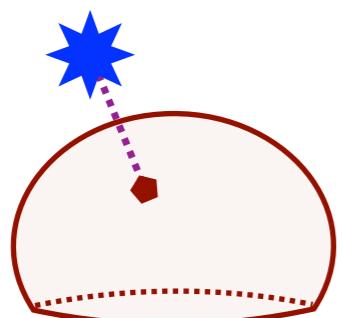
This Talk: Optimal Transport
Moult's Talk: Conformal Physics

These + Korchemsky's:
Energy Flow

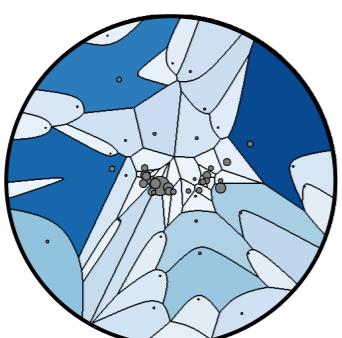
Outline



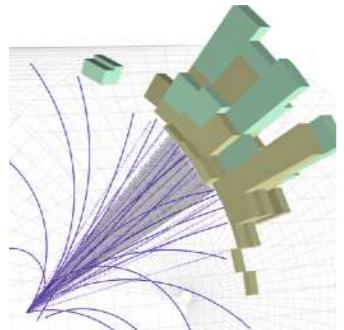
Going with the Flow



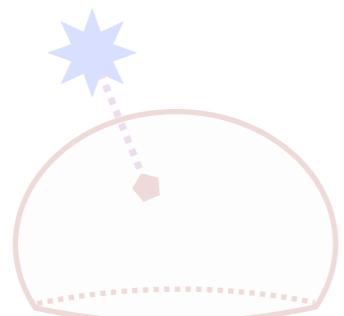
Flowing into the Past



Flowing into the Future



Going with the Flow



Flowing into the Past

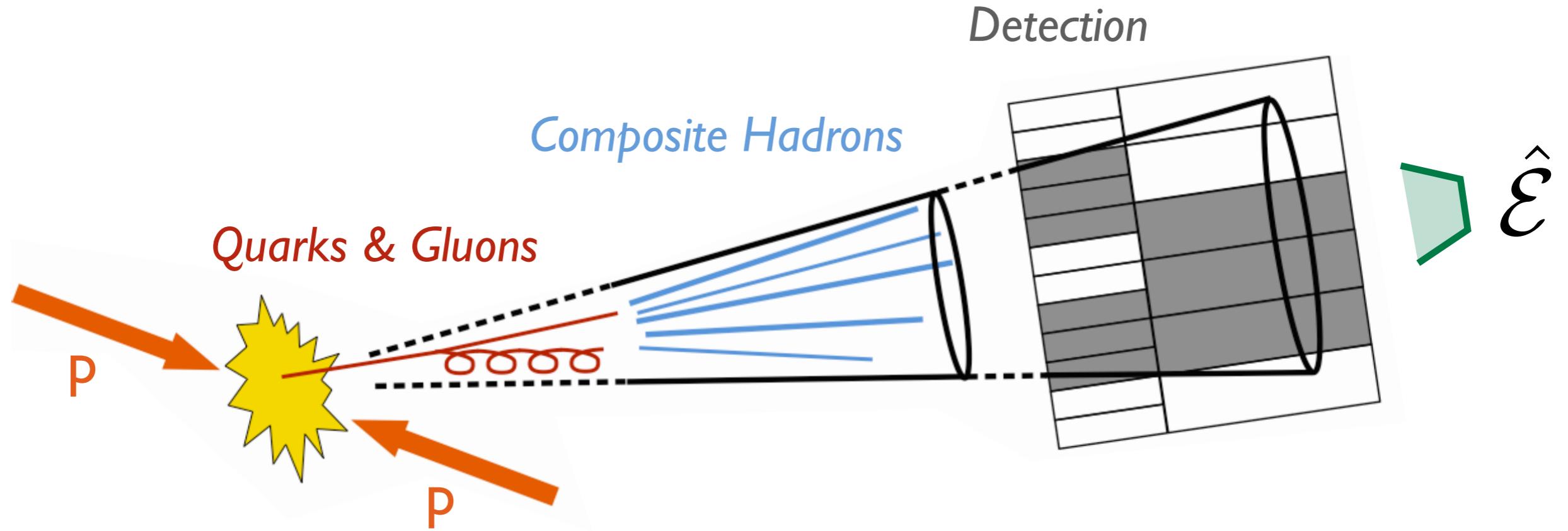


Flowing into the Future

Energy Flow Representation

Manifest *infrared and collinear safety*

Theory



Energy Flow:

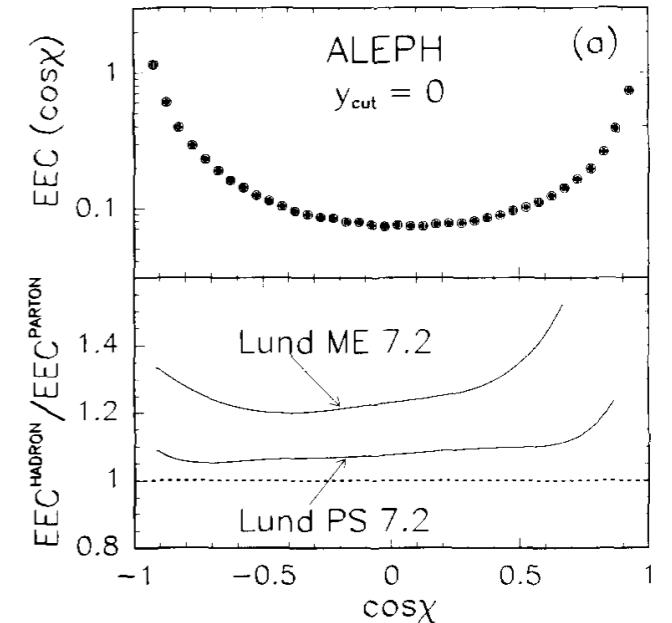
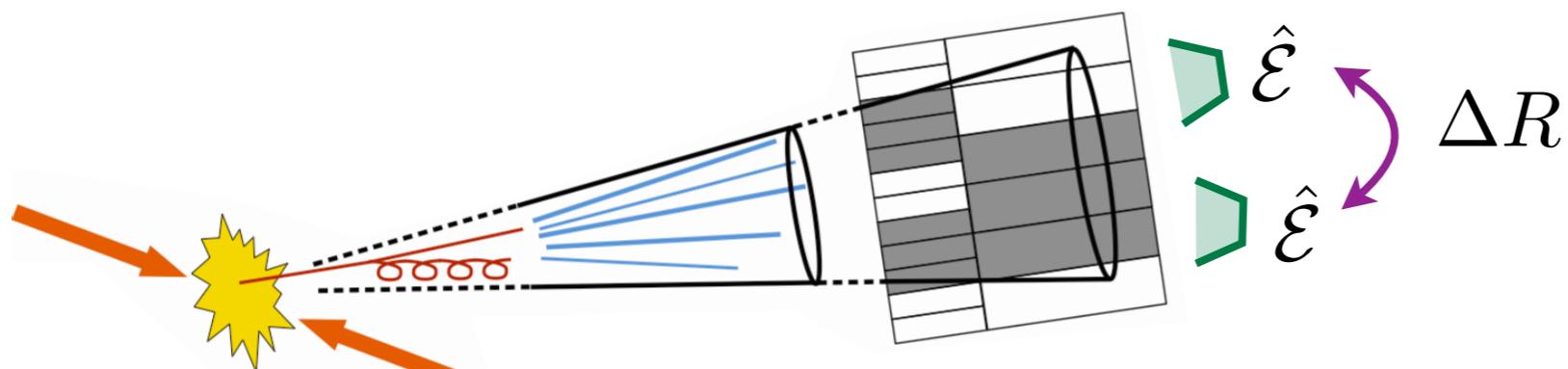
Robust to hadronization and detector effects
Well-defined for massless gauge theories

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

[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 probing the collinear dynamics of QCD:



A new chapter leveraging insights from the conformal limit!

Preview of Ian Moult's talk tomorrow:



[Basham, Brown, Ellis, Love, [PRL 1978](#); ALEPH, [PLB 1991](#)]
[cf. [Ian Moult's Inspire page](#); Komiske, Moult, JDT, Zhu, [arXiv 2022](#)]



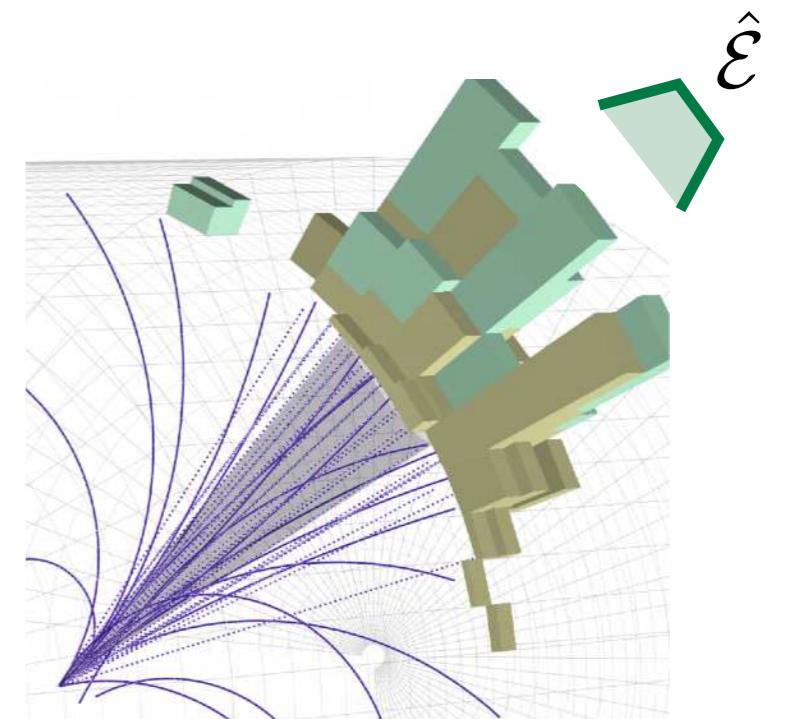
ML Perspective: Jets as **Weighted Point Clouds**

- **Energy-Weighted Directions**

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

↑ ━━
Energy Direction

(suppressing unsafe charge/flavor information)



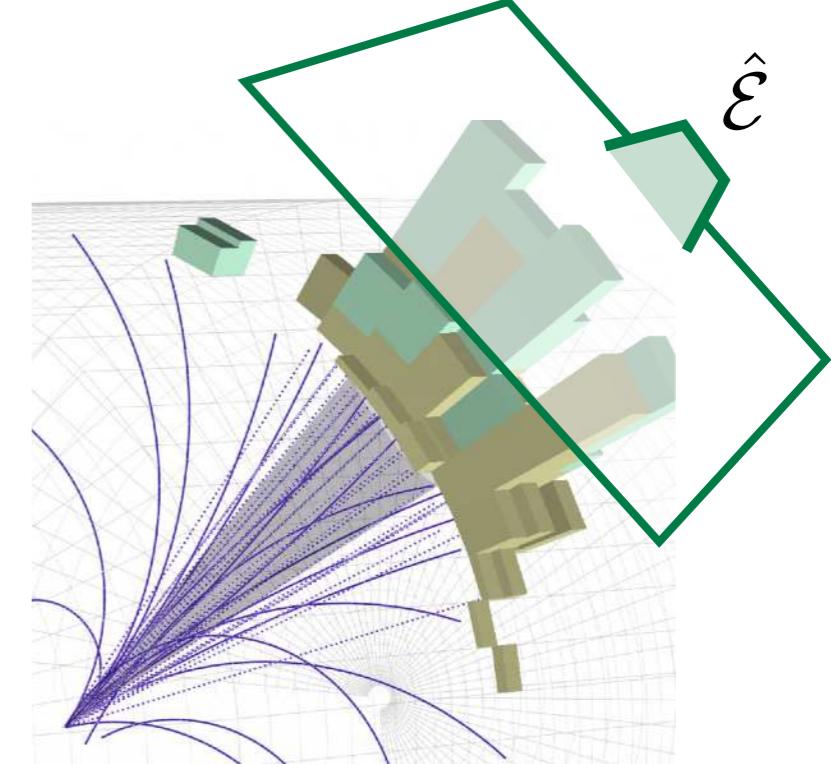
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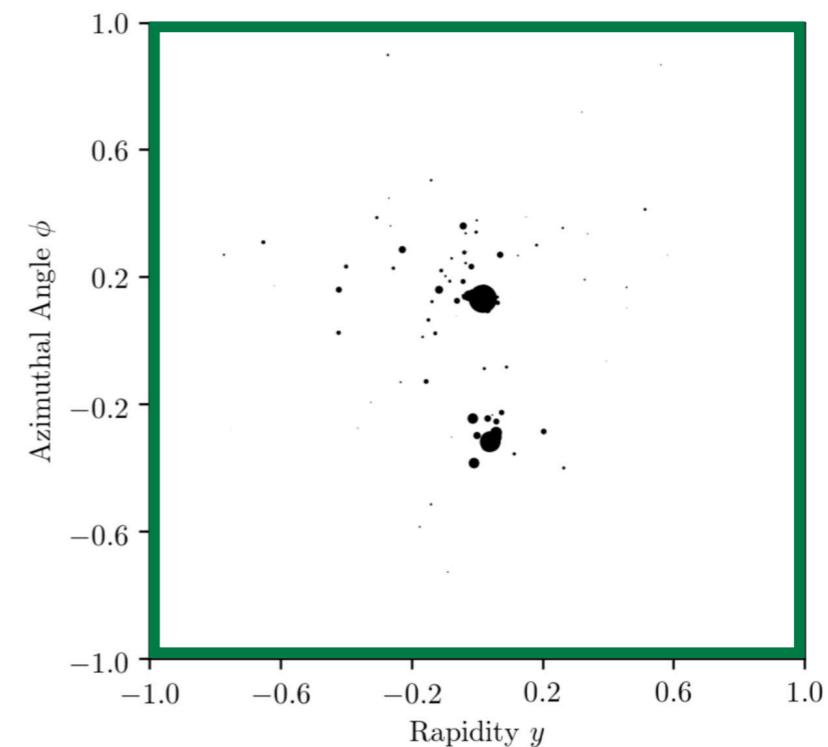
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- Equivalently: Energy Density

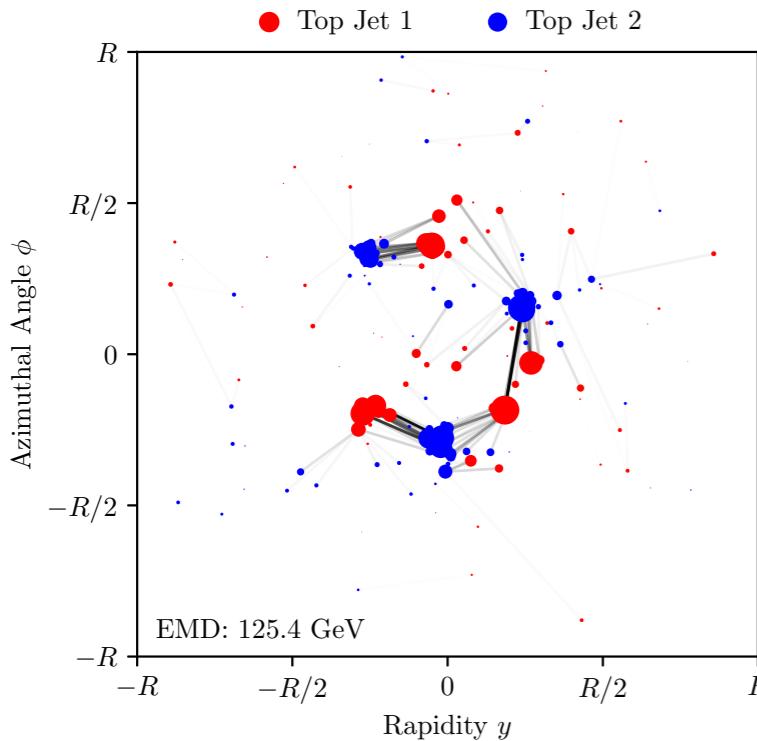
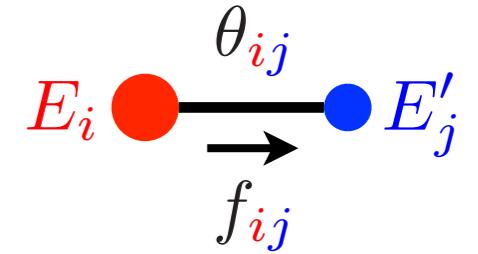
$$\rho(\hat{n}) = \sum_{i \in \mathcal{J}} E_i \delta^{(2)}(\hat{n} - \hat{n}_i)$$

↑ ↑
Energy Direction



The Energy Mover's Distance

Adapted from earth mover's distance of computer vision



Optimal transport between energy flows...

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

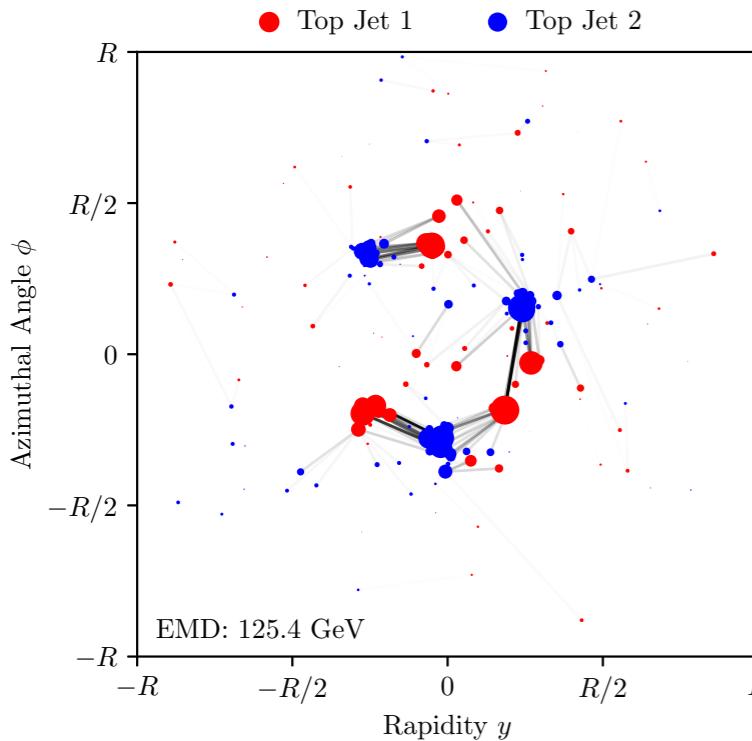
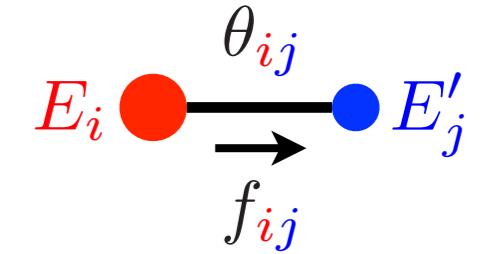
↑
in GeV Cost to move energy Cost to create energy

[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/unbalanced transport in Cai, Cheng, Craig, Craig, [PRD 2020, arXiv 2021](#)]



The Energy Mover's Distance

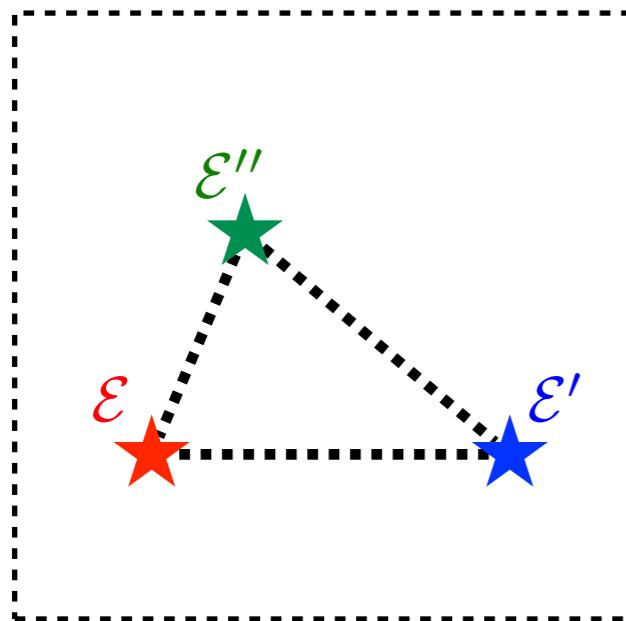
Adapted from earth mover's distance of computer vision



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

↑
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](#);

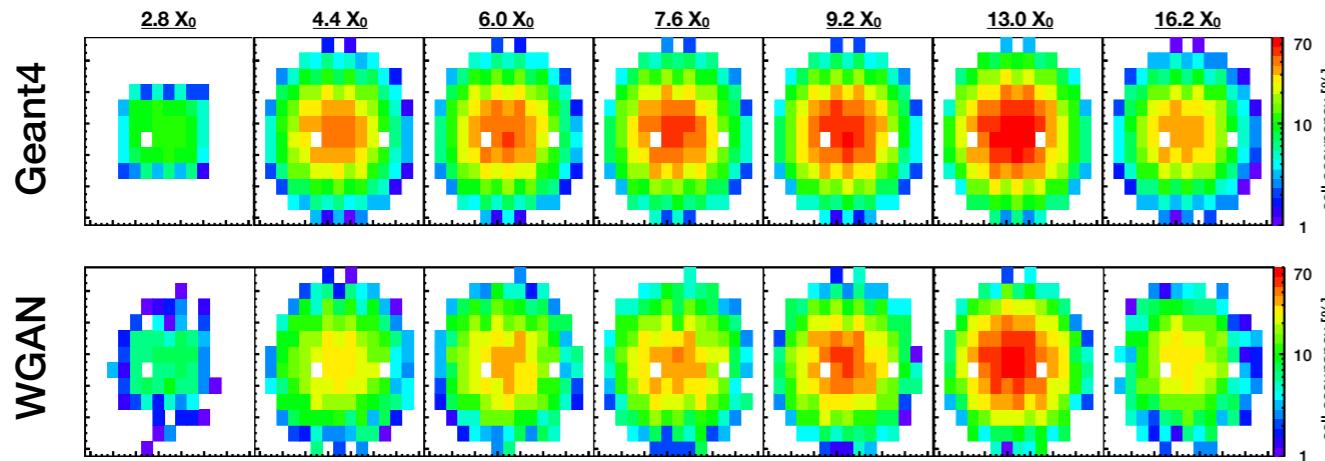
[see flavored variant in Crispim Romão, Castro, Milhano, Pedro, Vale, [EPJC 2021](#)]

[see computational speed up/unbalanced transport in Cai, Cheng, Craig, Craig, [PRD 2020](#), [arXiv 2021](#)]



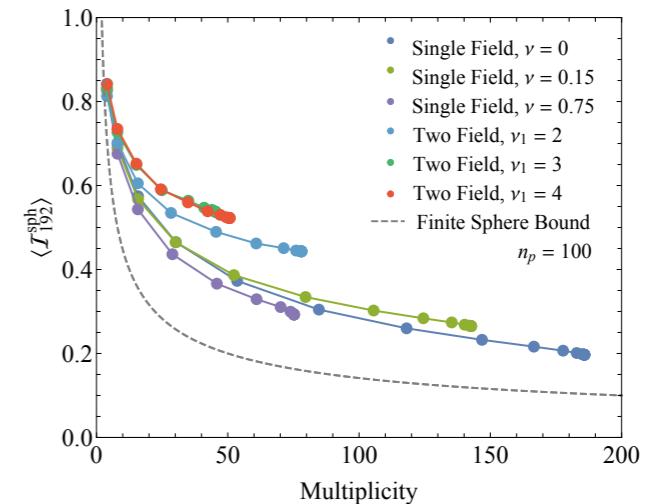
Wasserstein Elsewhere in HEP

Generative Modeling



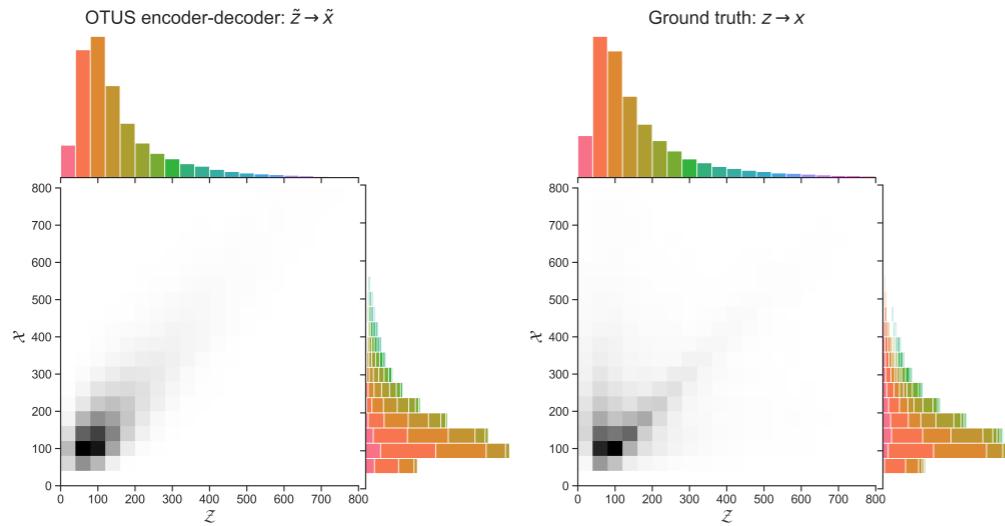
[Erdmann, Geiger, Glombitza, Schmidt, [CSBS 2018](#); Erdmann, Glombitza, Quast, [CSBS 2019](#);
Chekalina, Orlova, Ratnikov, Ulyanov, Ustyuzhanin, Zakharov, [CHEP 2018](#)]

BSM Characterization



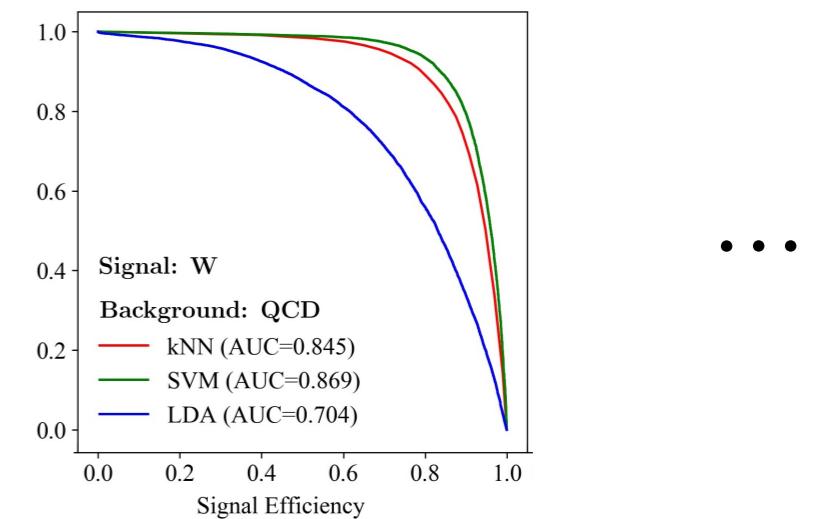
[Cesarotti, Reece, Strassler, [JHEP 2021](#), [arXiv 2020](#)]

Estimated Simulation/Unfolding

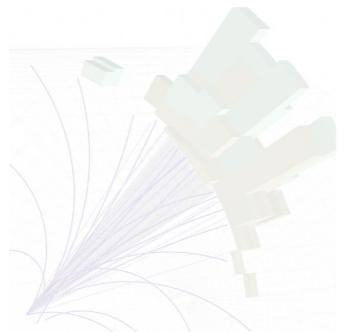


[Howard, Mandt, Whiteson, Yang, [arXiv 2021](#)]

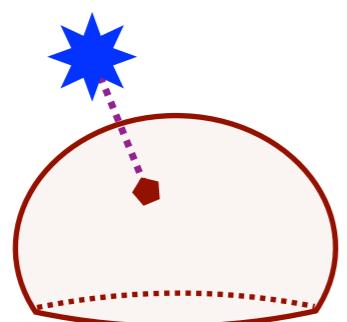
Jet Classification



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



Going with the Flow



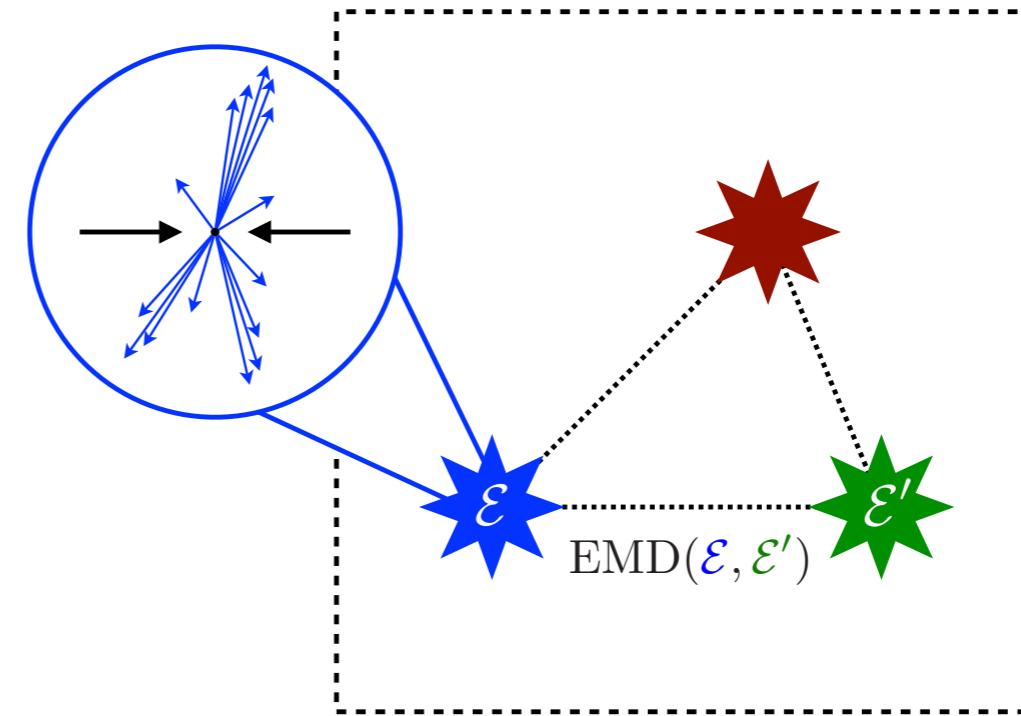
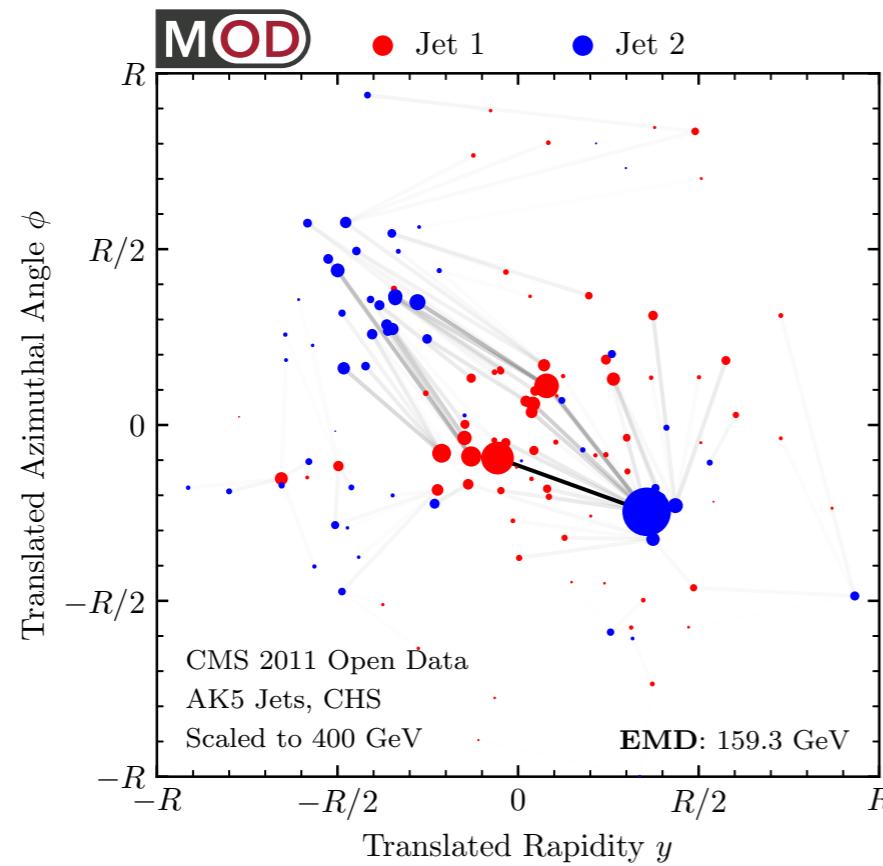
Flowing into the Past



Flowing into the Future

Optimal Transport for Collider Geometry

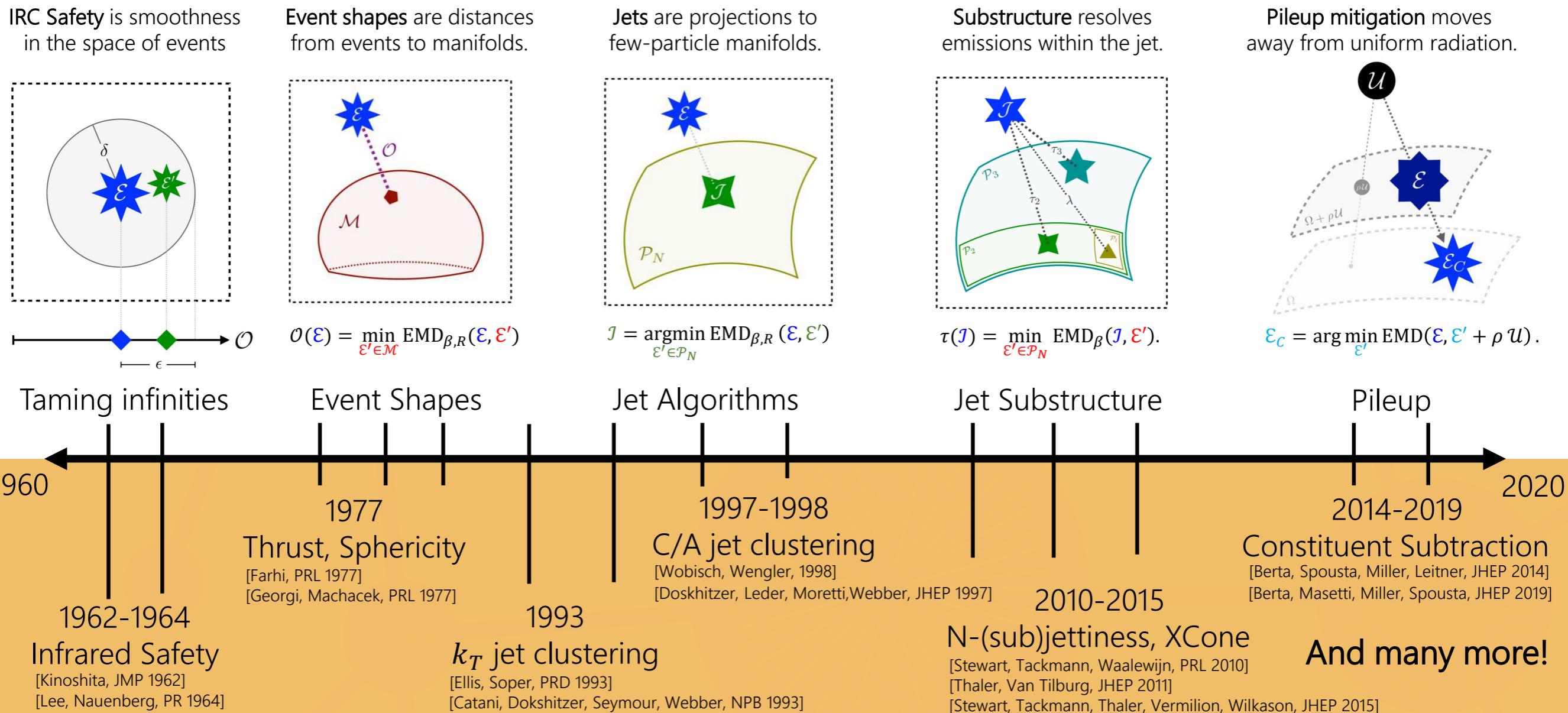
Energy Mover's Distance \Rightarrow Metric Space of Collider Events



New insights into high-energy physics facilitated by advances in mathematics, statistics, and computer science

[Komiske, Metodiev, JDT, [PRL 2019](#); code at [Komiske, Metodiev, JDT, energyflow.network](#); open data study in Komiske, Mastandrea, Metodiev, Naik, JDT, [PRD 2020](#)] [based on Peleg, Werman, Rom, [IEEE 1989](#); Rubner, Tomasi, Guibas, [ICCV 1998](#), [ICJV 2000](#); Pele, Werman, [ECCV 2008](#); Pele Taskar, [GSI 2013](#)]

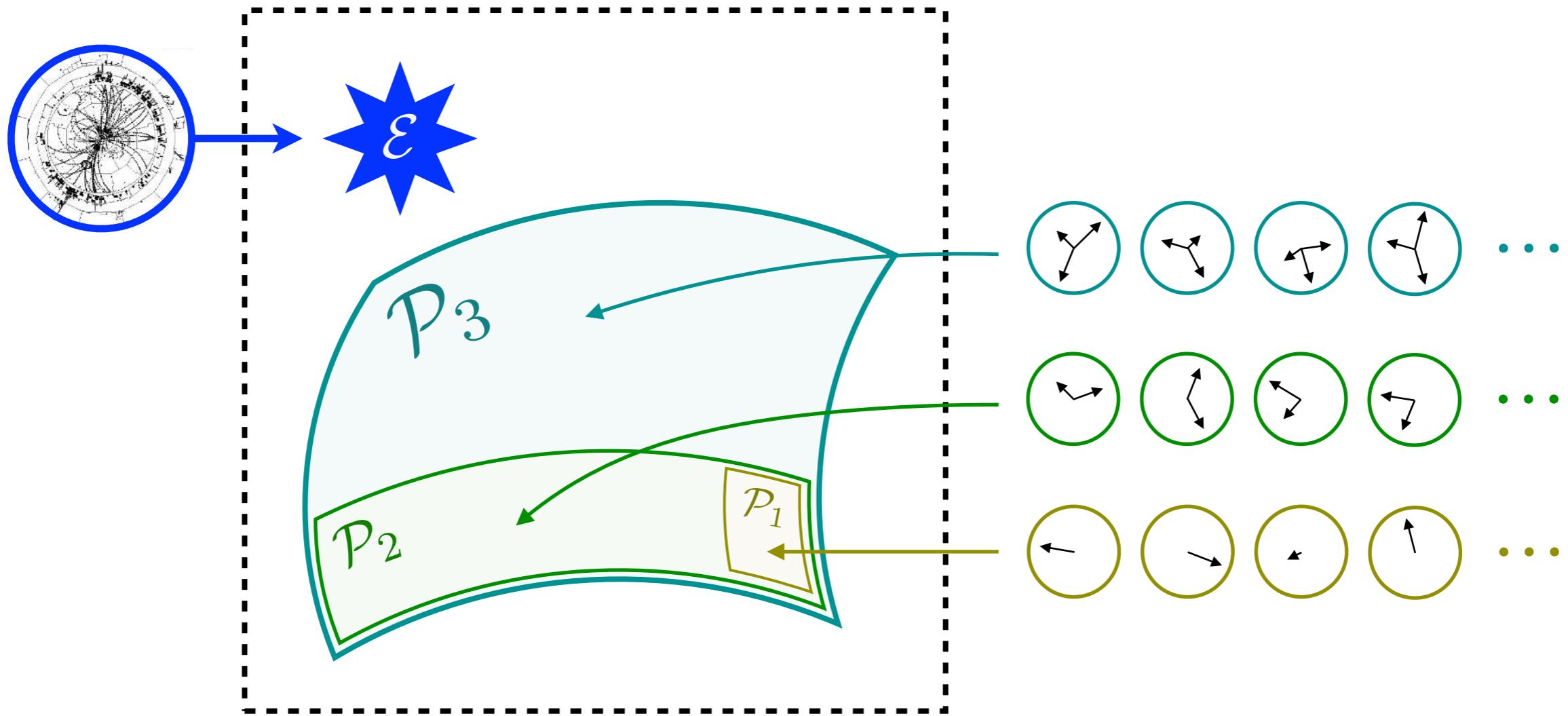
Six Decades of Collider Physics Translated into a New Geometric Language!



[Timeline from Eric Metodiev]

Introducing N-particle Manifolds

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

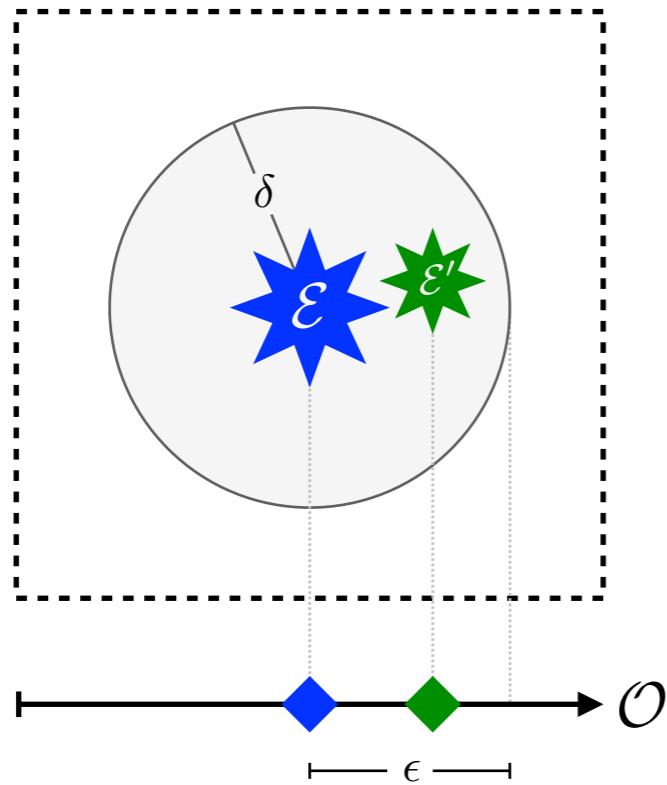


$\mathcal{P}_N \supset \mathcal{P}_{N-1} \supset \dots \supset \mathcal{P}_2 \supset \mathcal{P}_1$ by soft/collinear limits

[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]

Observable Taxonomy

See backup for
example observables

All Observables

Measurable at a collider

Defined on Energy Flows

Invariant to exact infrared & collinear emissions everywhere except a negligible set of events

Infrared & Collinear Safe

EMD continuous everywhere except a negligible set of events

EMD Hölder Continuous

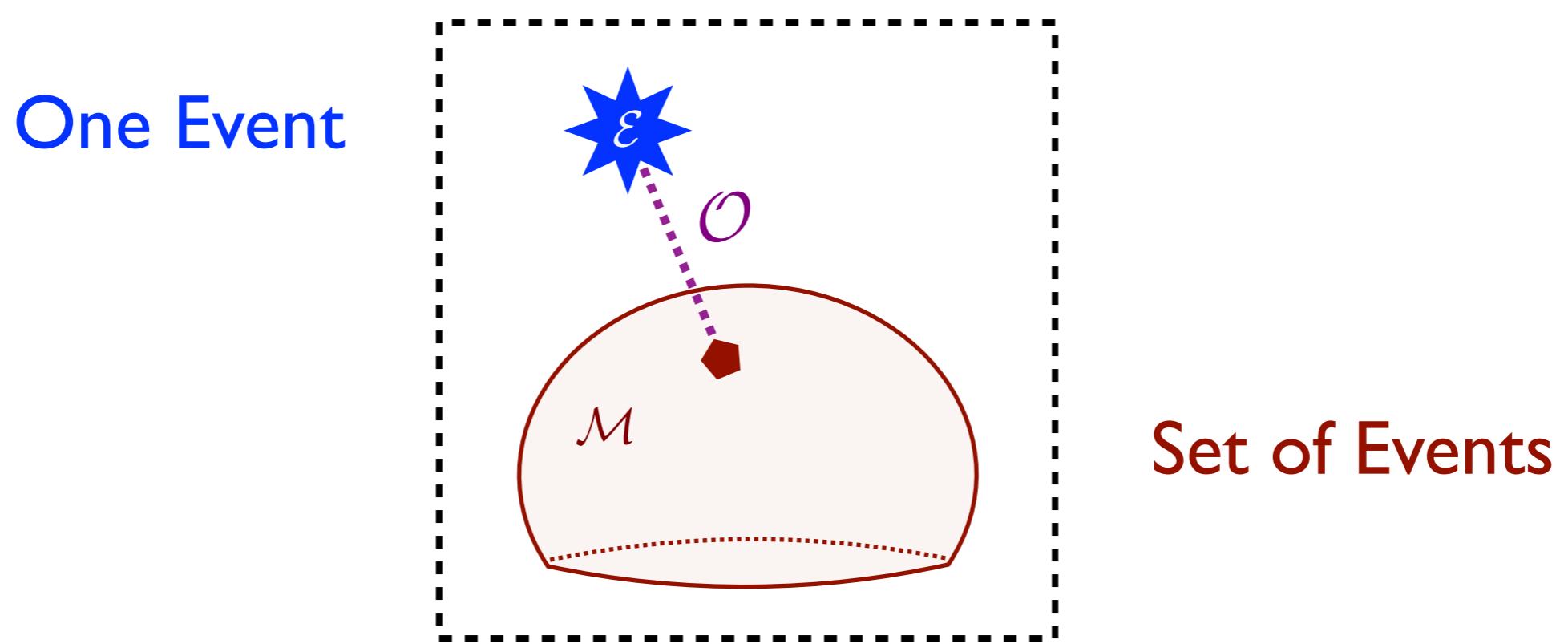
*Everywhere invariant to infinitesimal
infrared & collinear emissions*

Sudakov Safe

*Discontinuous on some
N-particle manifolds*

[Komiske, Metodiev, JDT, [JHEP 2020](#); cf. Sterman, [PRD 1979](#); Banfi, Salam, Zanderighi, [JHEP 2005](#); Larkoski, Marzani, JDT, [PRD 2015](#)]

Manifolds for Observables



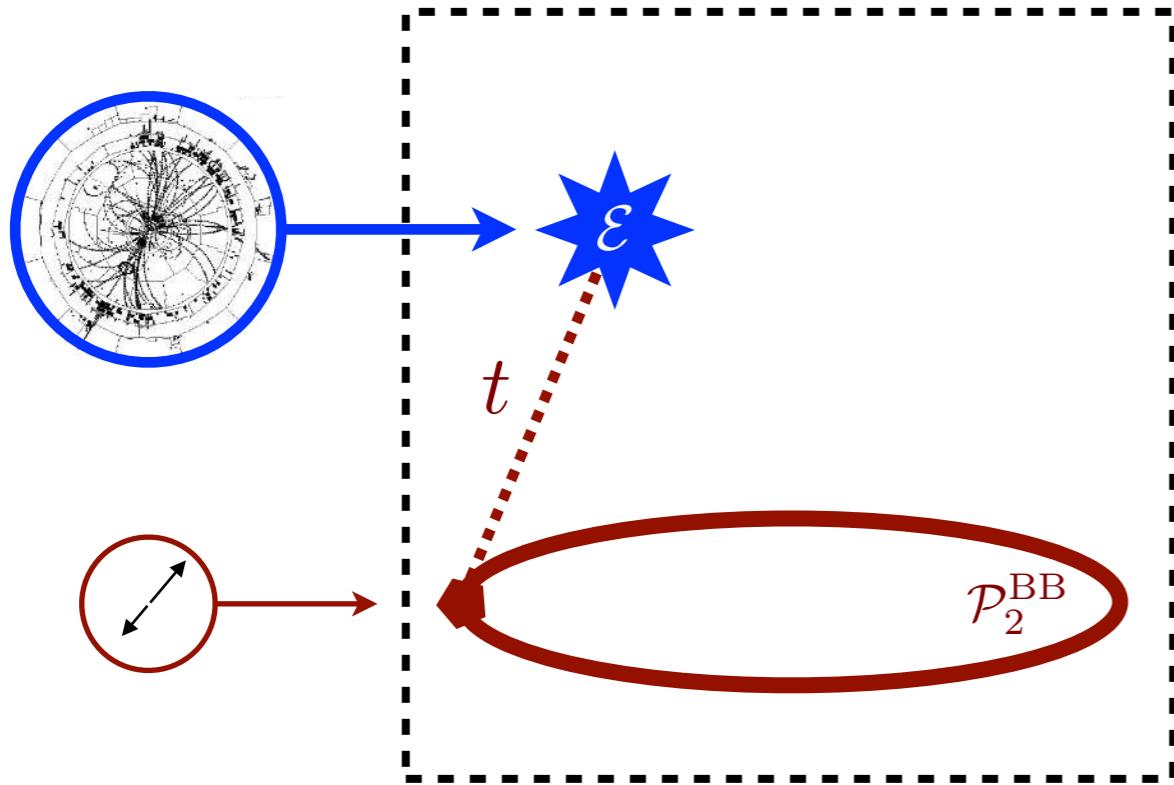
Distance of Closest Approach \Rightarrow Observable

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

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

E.g. Thrust

How dijet-like is an event?



All Back-to-Back Two Particle Configurations

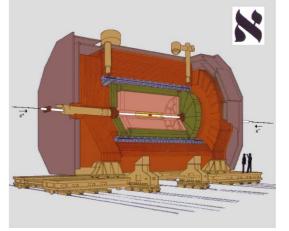
$$\mathcal{P}_2^{\text{BB}} = \left\{ \begin{array}{c} \text{red circle with arrows} \\ \cdots \end{array} \right\}$$

(using $\beta=2$ EMD variant)

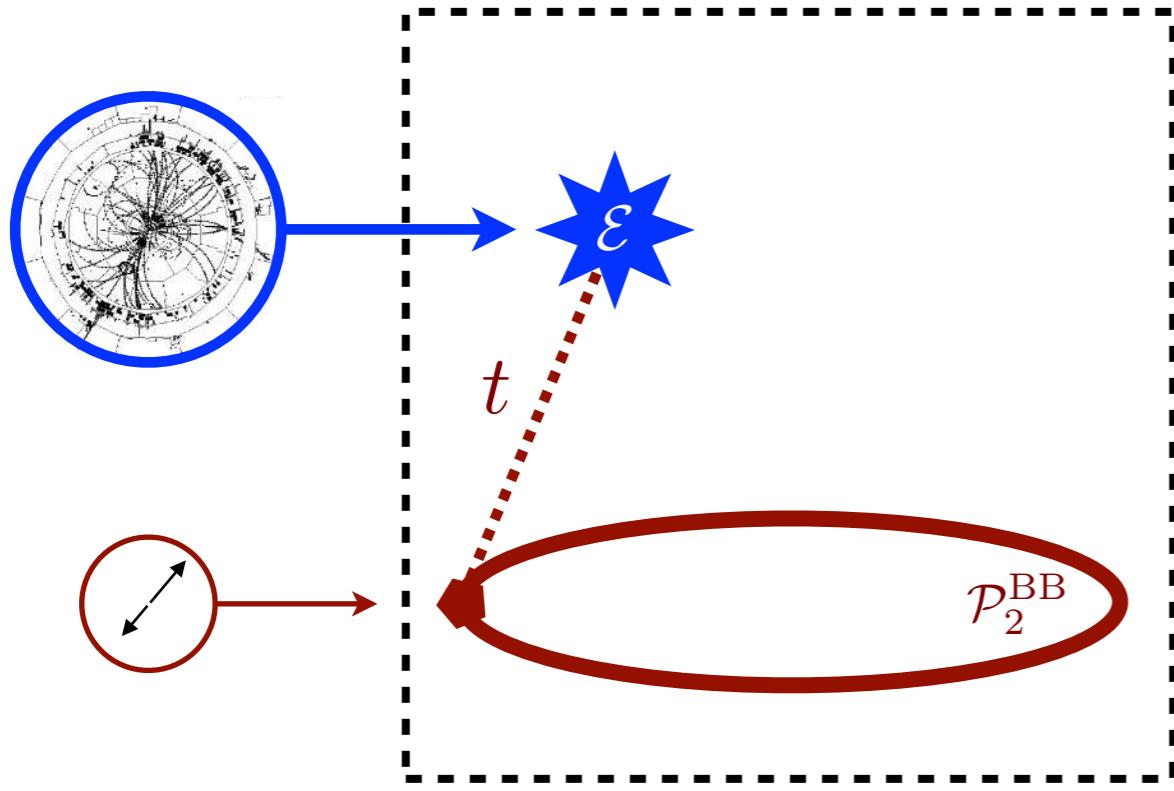
[Komiske, Metodiev, JDT, [JHEP 2020](#)
Brandt, Peyrou, Sosnowski, Wroblewski, [PL 1964](#); Farhi, [PRL 1977](#); ALEPH, [PLB 1991](#)]

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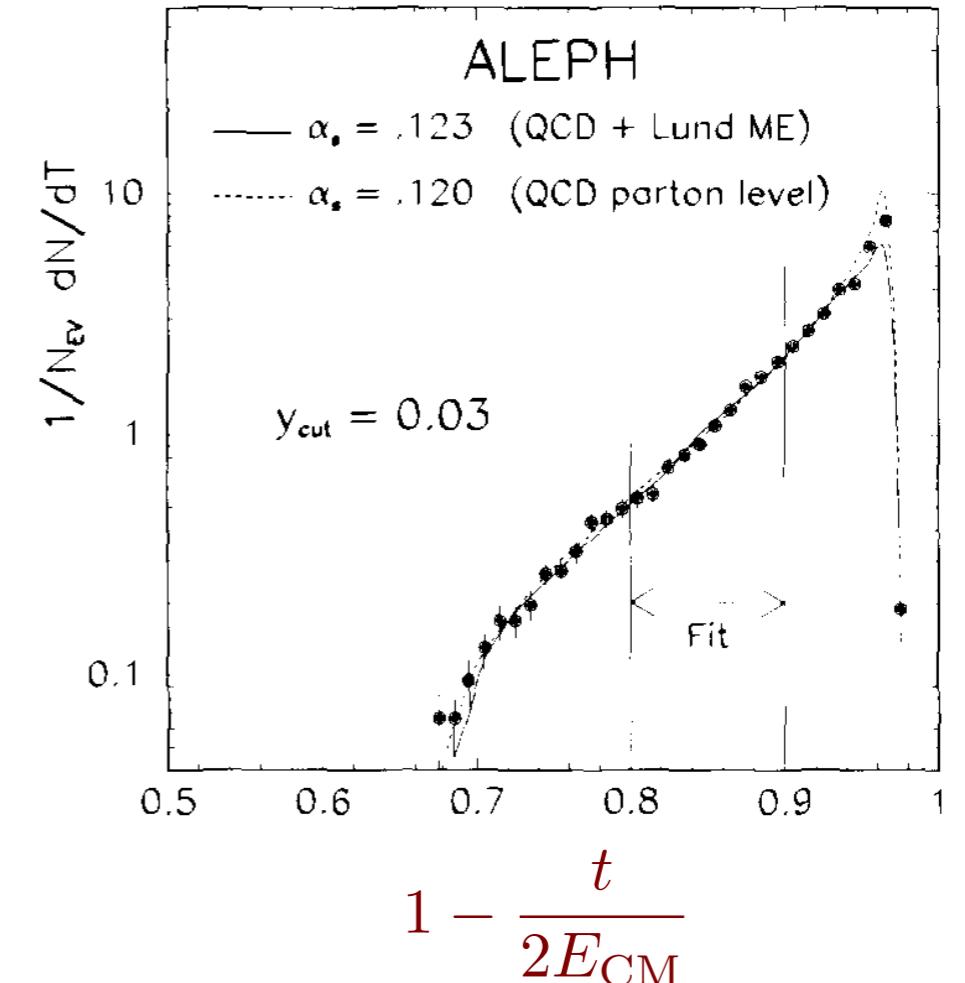
$$t(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{P}_2^{\text{BB}}} \text{EMD}_2(\mathcal{E}, \mathcal{E}')$$



All Back-to-Back Two Particle Configurations

$$\mathcal{P}_2^{\text{BB}} = \left\{ \begin{array}{c} \text{red circle with two arrows pointing away} \\ \text{red circle with two arrows pointing towards} \\ \text{red circle with one arrow pointing up} \\ \text{red circle with one arrow pointing down} \\ \cdots \end{array} \right\}$$

(using $\beta=2$ EMD variant)



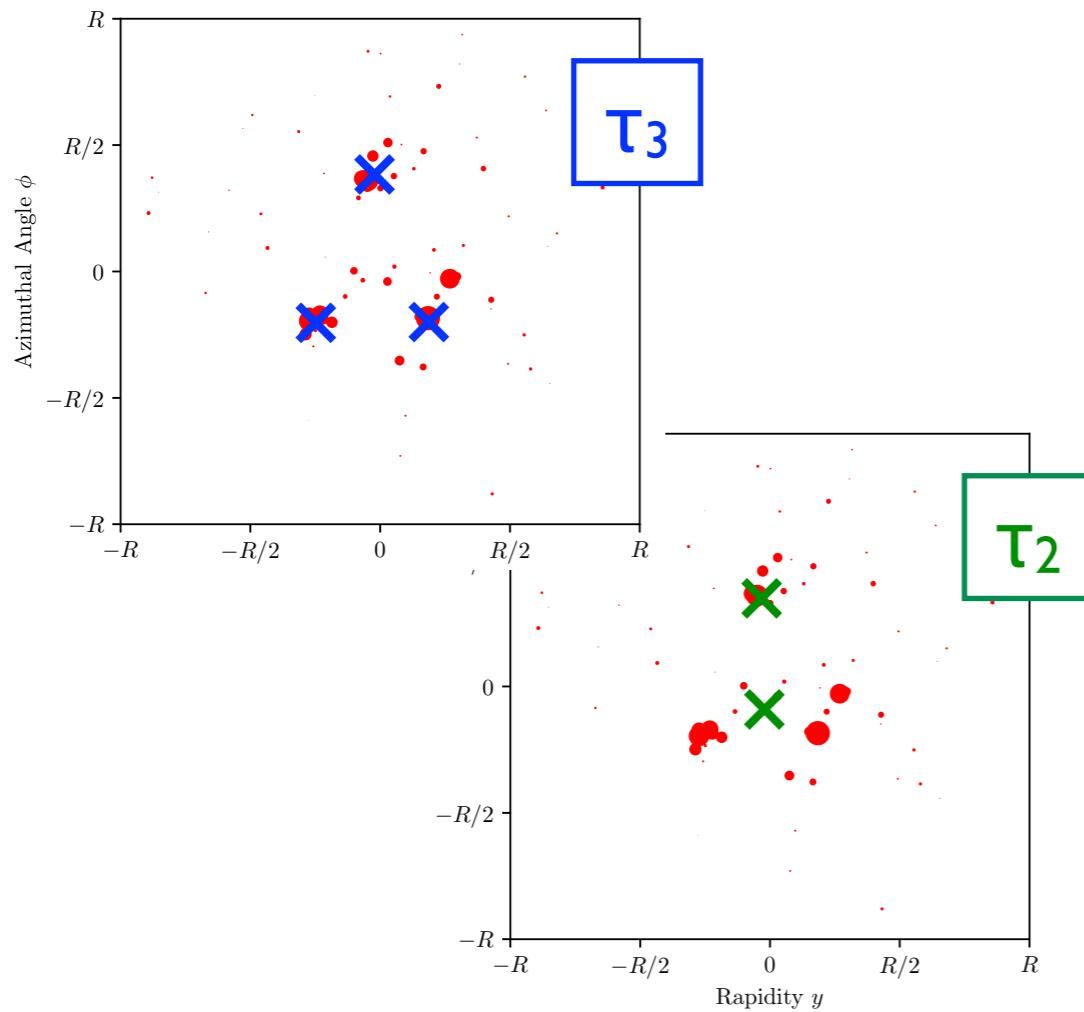
$$\text{cf. } T(\mathcal{E}) = \max_{\hat{n}} \frac{\sum_i |\vec{p}_i \cdot \hat{n}|}{\sum_j |\vec{p}_j|}$$

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

N-subjettiness

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

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



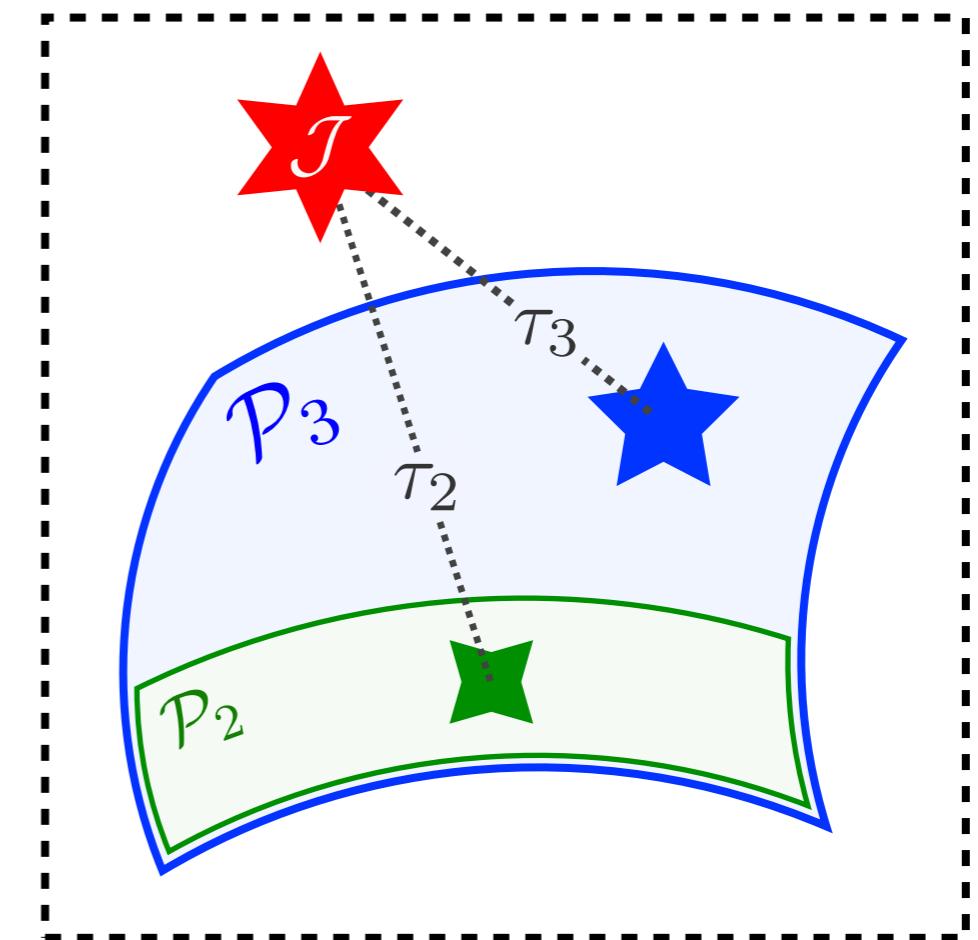
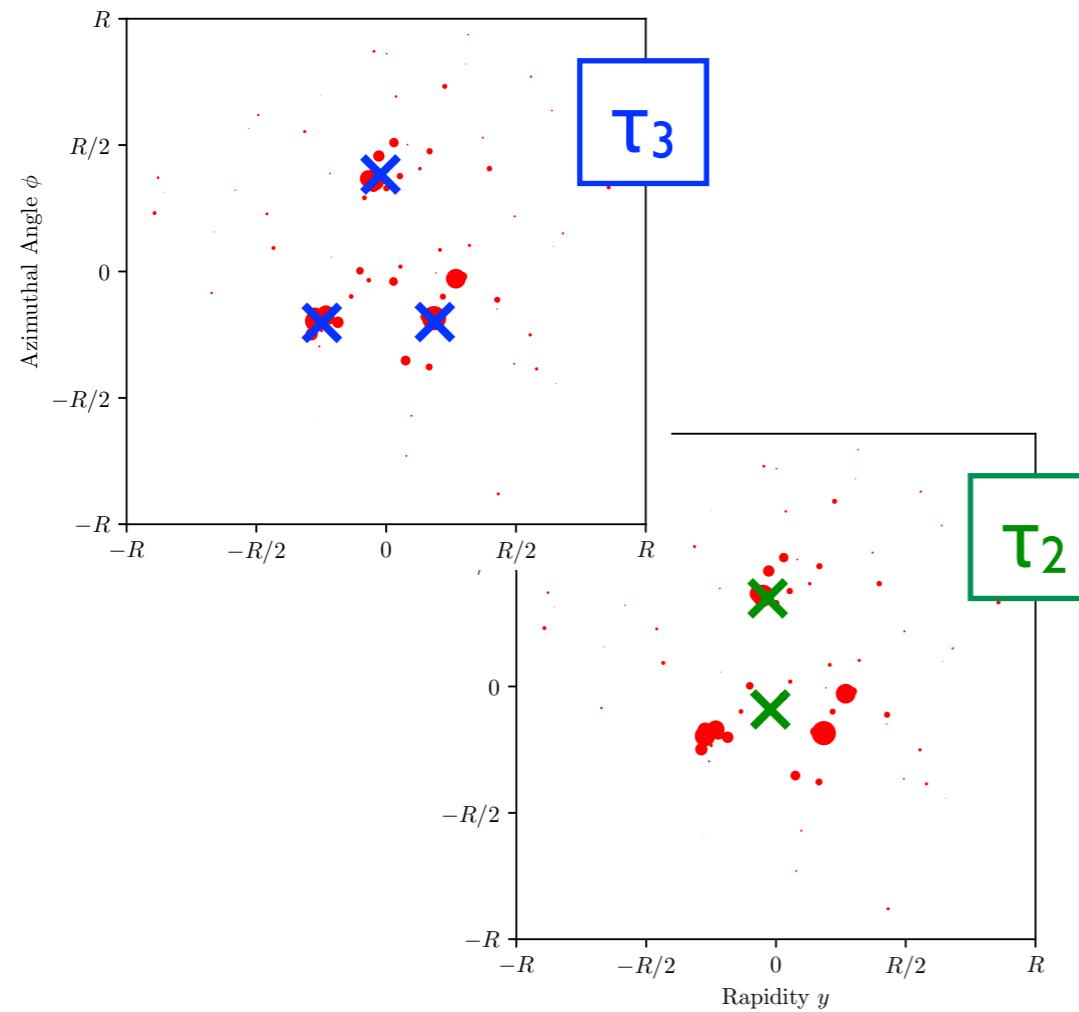
[JDT, Van Tilburg, [JHEP 2011](#), [JHEP 2012](#);
based on Brandt, Dahmen, [ZPC 1979](#); Stewart, Tackmann, Waalewijn, [PRL 2010](#)]



N-subjettiness = Point to Manifold EMD

...is secretly an optimal transport problem

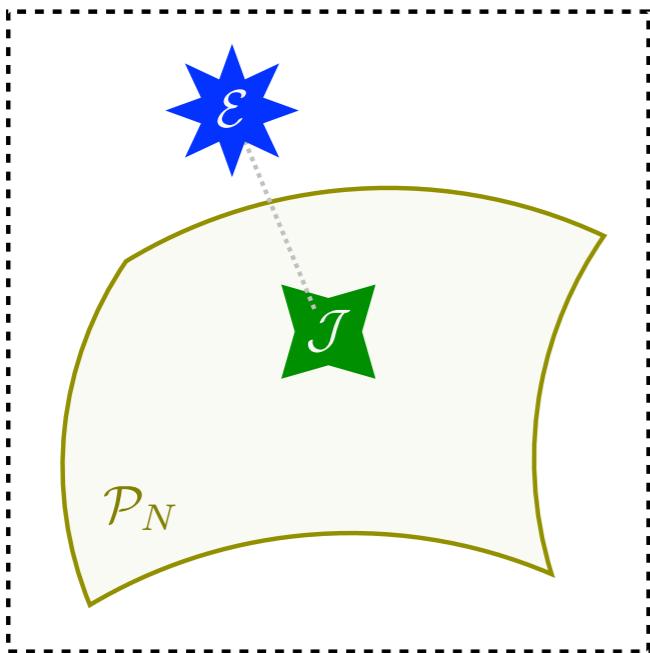
$$\tau_N(\mathcal{J}) = \min_{\mathcal{J}' \in \mathcal{P}_N} \text{EMD}(\mathcal{J}, \mathcal{J}')$$



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



More Fun with N-particle Manifolds



N-jettiness

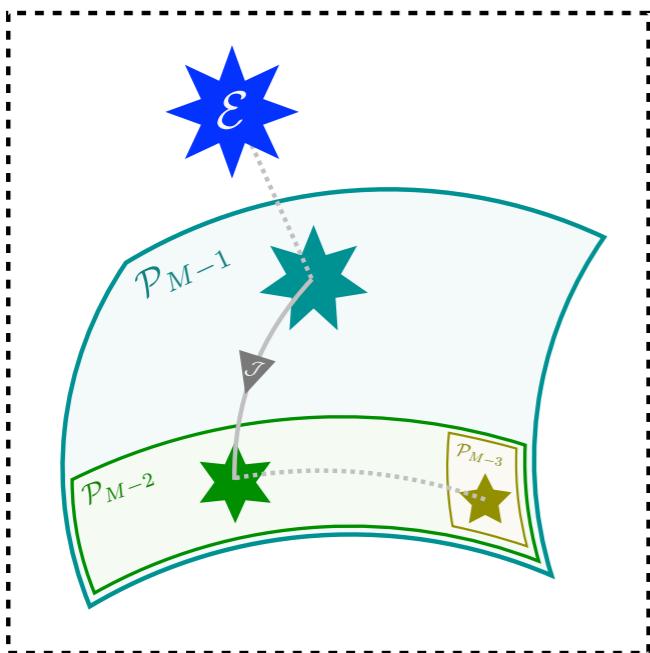
Distance of closest approach to N-particle manifold

[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

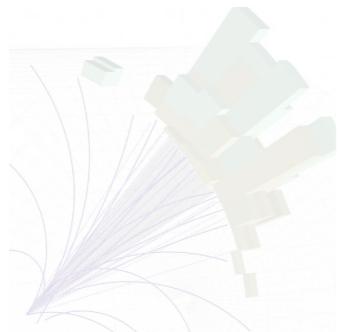
Iteratively stepping between various N-particle manifolds

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

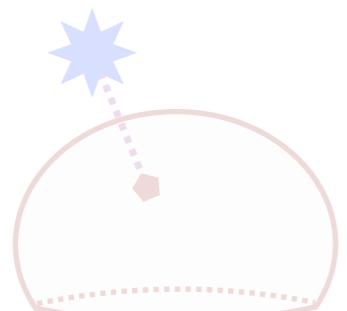
[Dokshitzer, Leder, Moretti, Webber, [JHEP 1997](#); Wobisch, Wengler, [arXiv 1999](#)]

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

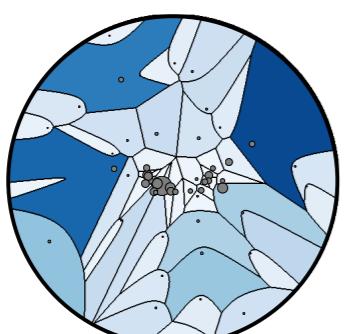
[Komiske, Metodiev, JDT, [JHEP 2020](#)]



Going with the Flow



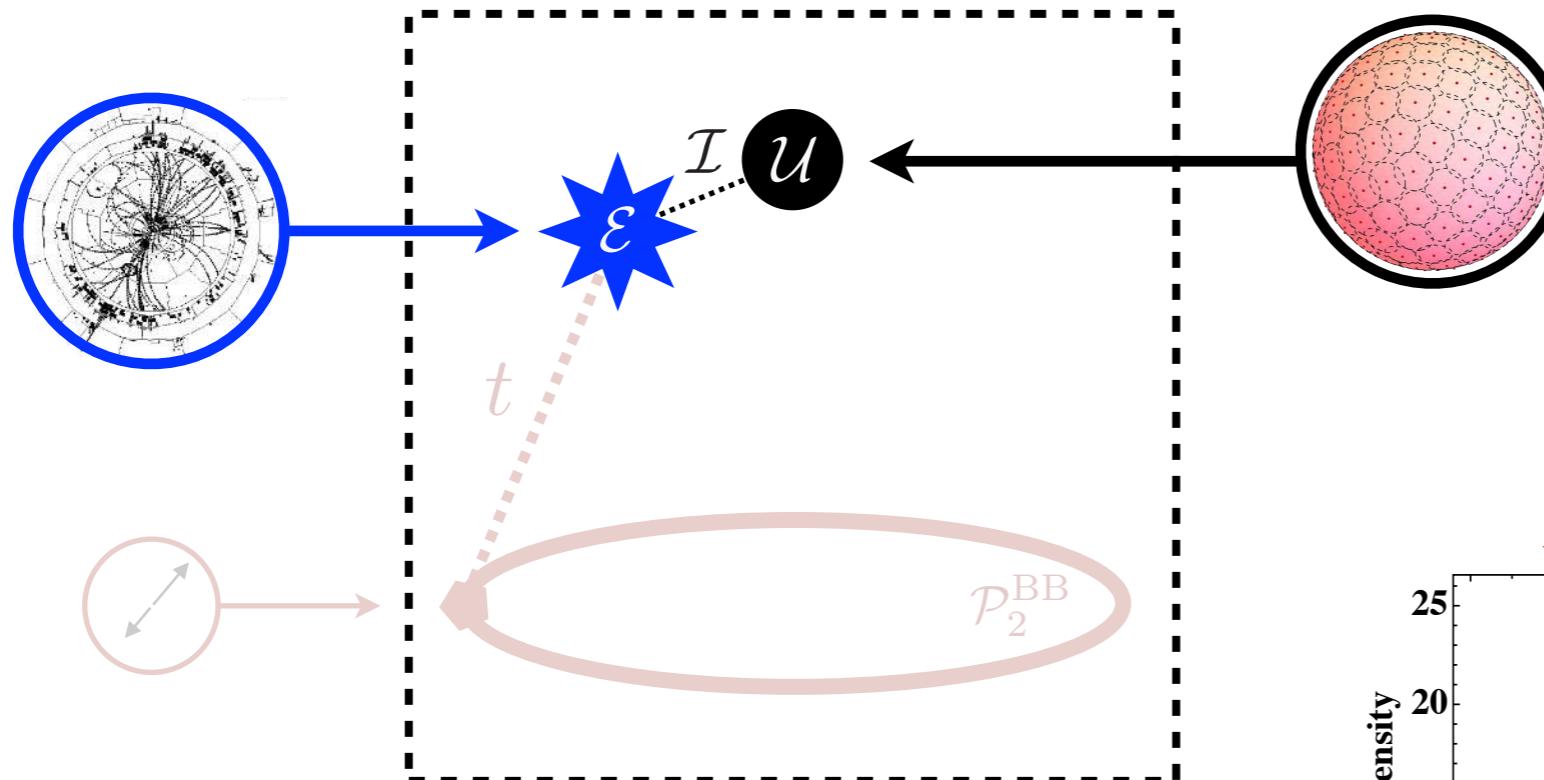
Flowing into the Past



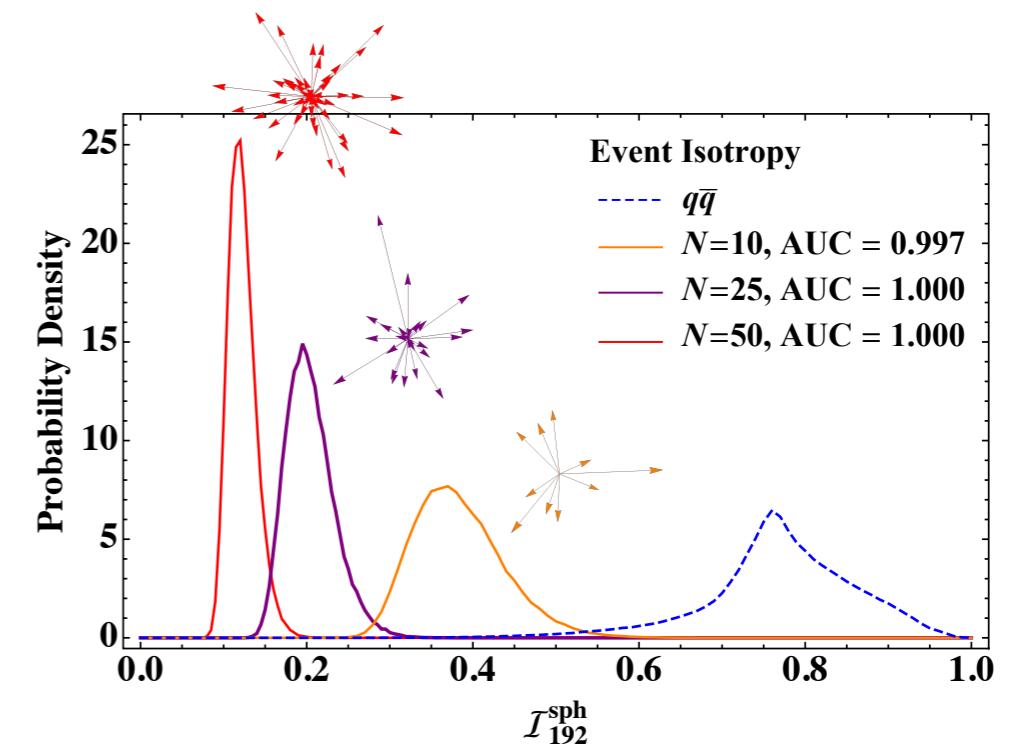
Flowing into the Future

New! Event Isotropy

How isotropic is an event?



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



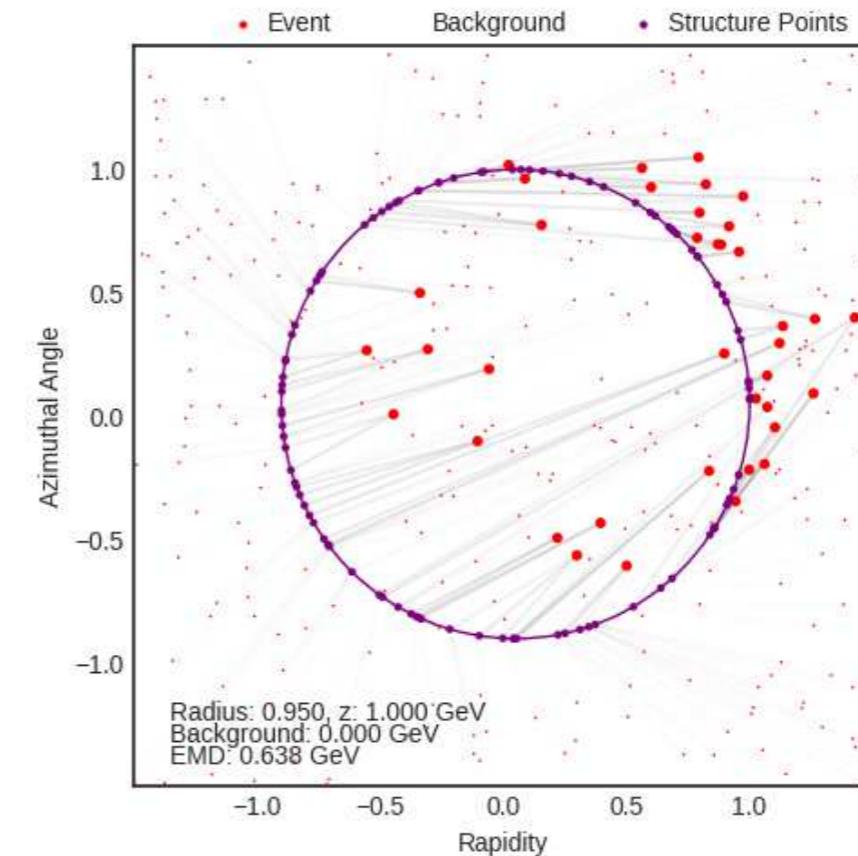
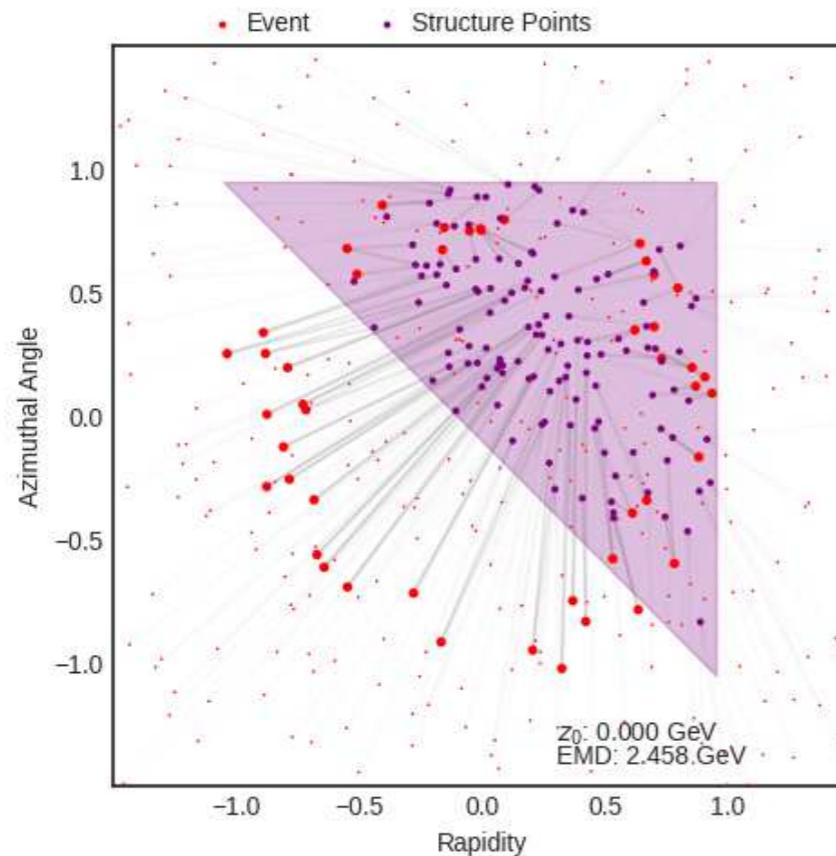
[Cesarotti, JDT, [JHEP 2020](#);
see also Cesarotti, Reece, Strassler, [JHEP 2021](#)]



Deep Manifold Learning

Optimal transport meets gradient descent

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

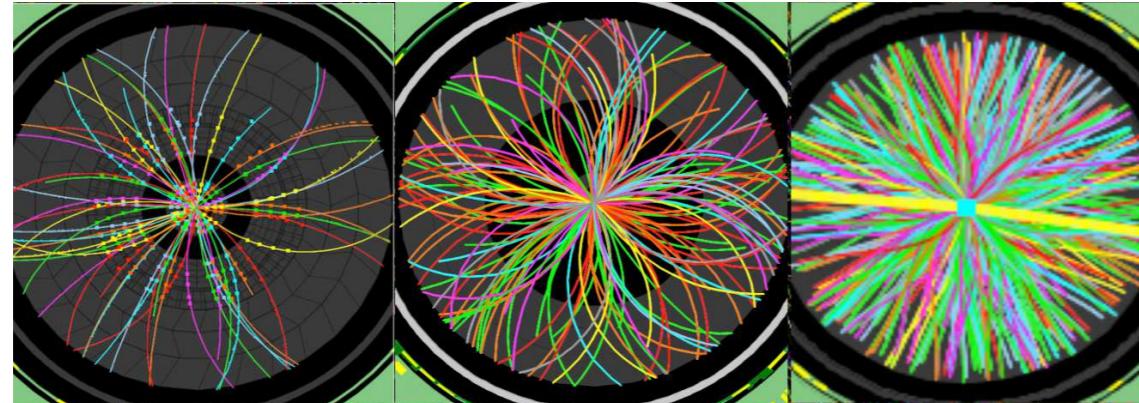


$$\mathcal{O}(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{M}} \text{EMD}(\mathcal{E}, \mathcal{E}')$$

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

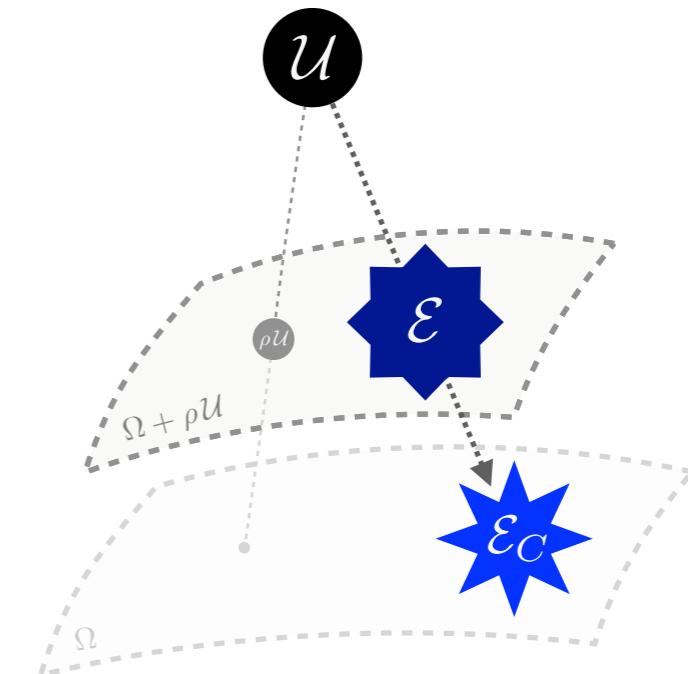


Pileup Mitigation



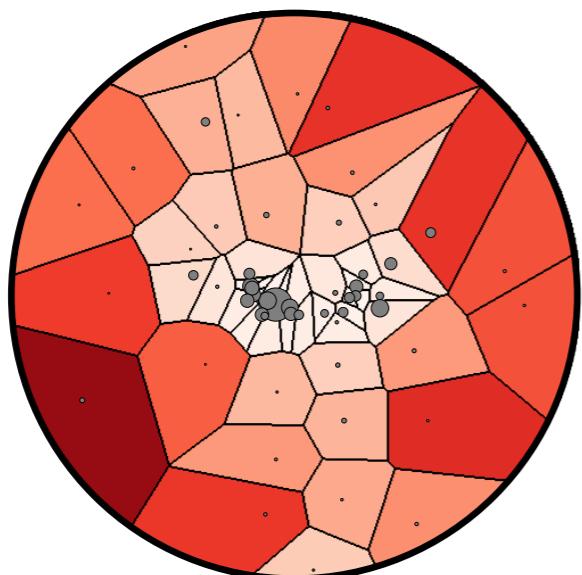
[see review in Soyez, PR 2019]

Uniform event contamination from overlapping proton-proton collisions



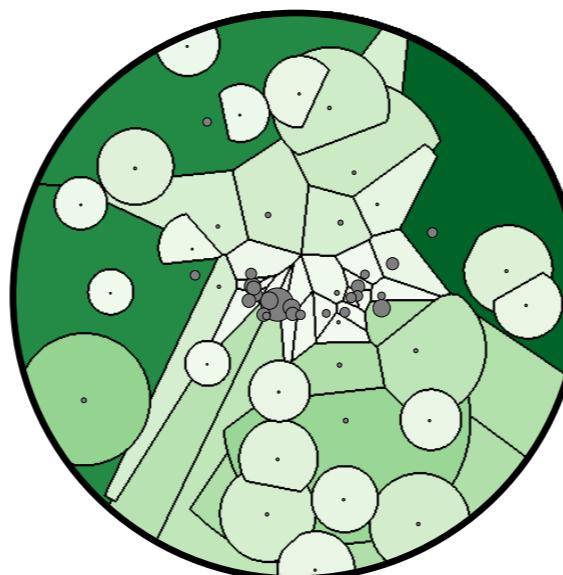
Pileup Mitigation:
“Move away” from uniform event

Voronoi



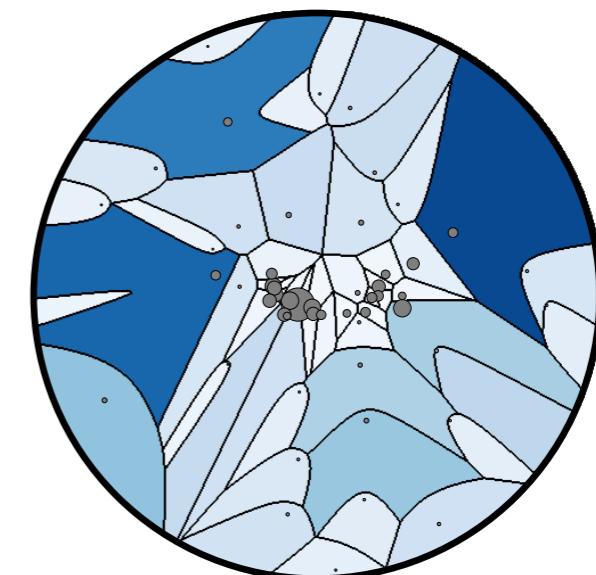
[Cacciari, Salam, Soyez, JHEP 2008]

Constituent Subtraction



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

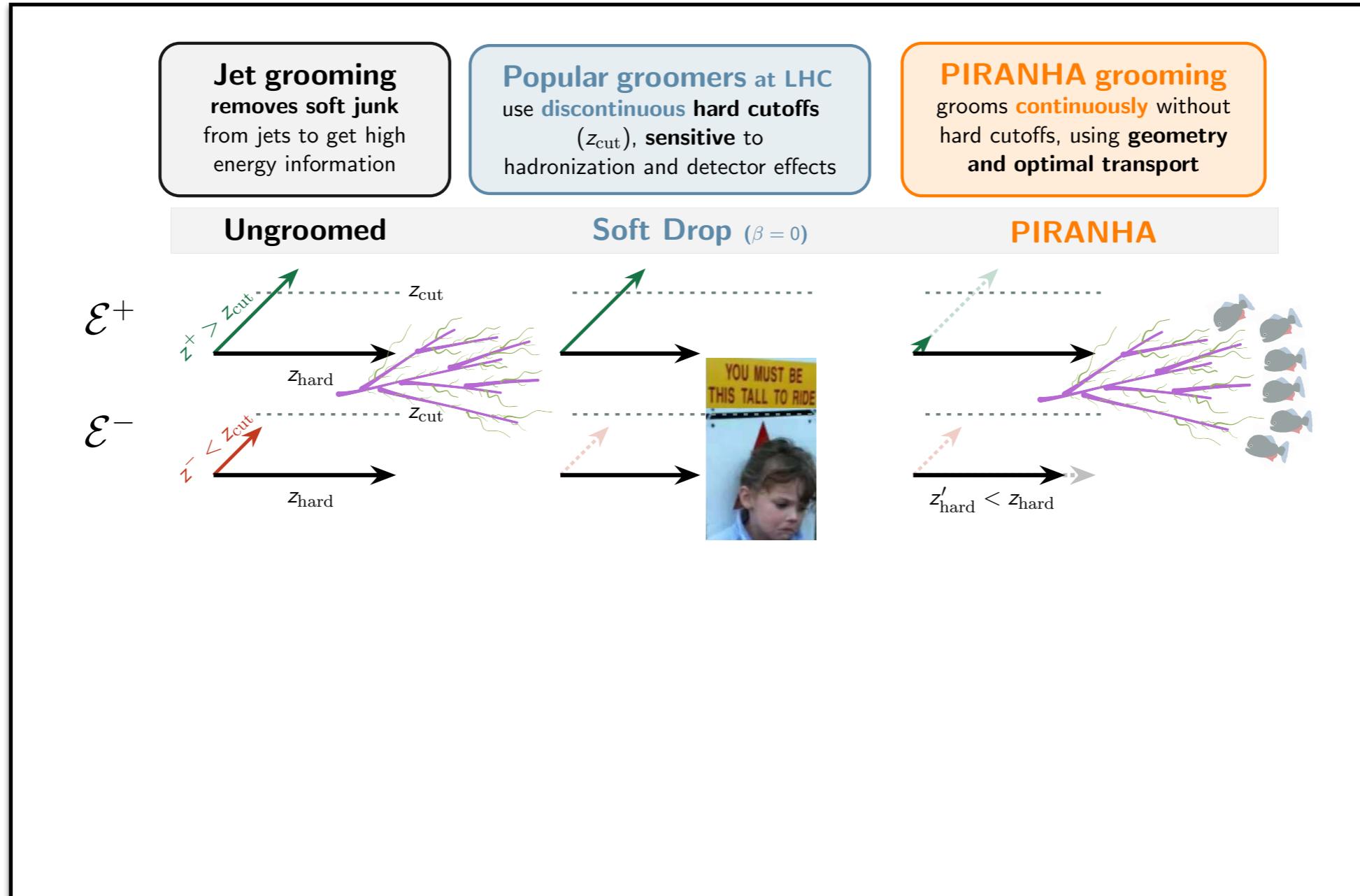
Apollonius



[Komiske, Metodiev, JDT, JHEP 2020]

Pileup and Infrared Radiation AnNiHilAtion

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

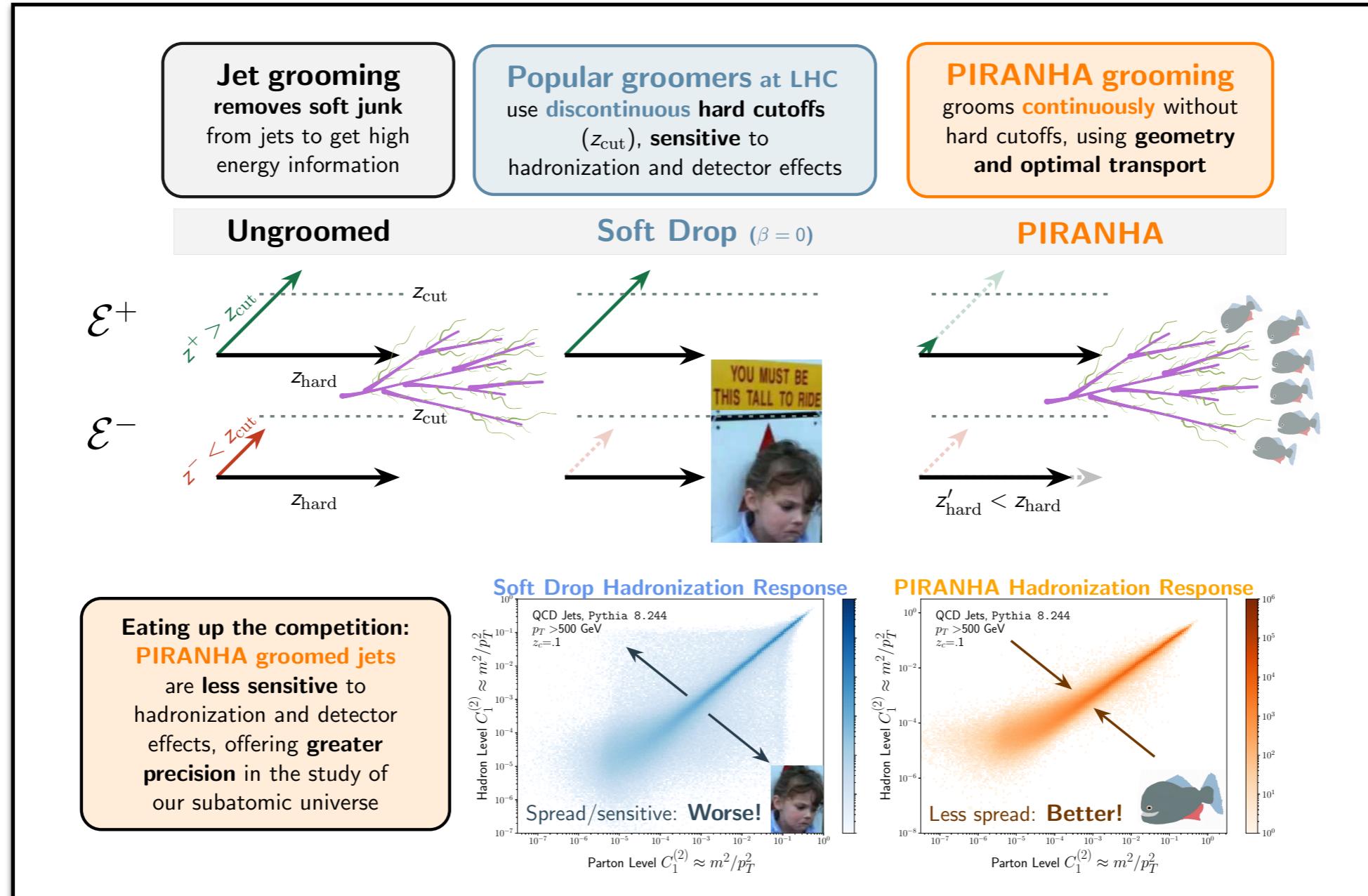


[Slides from Sam Alipour-fard]
[Alipour-fard, Komiske, Metodiev, JDT, in progress]



Pileup and Infrared Radiation AnNiHilAtion

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



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

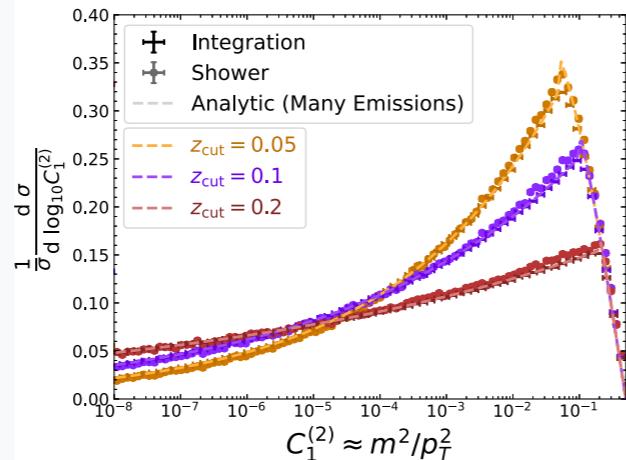


Pileup and Infrared Radiation AnNiHilAtion

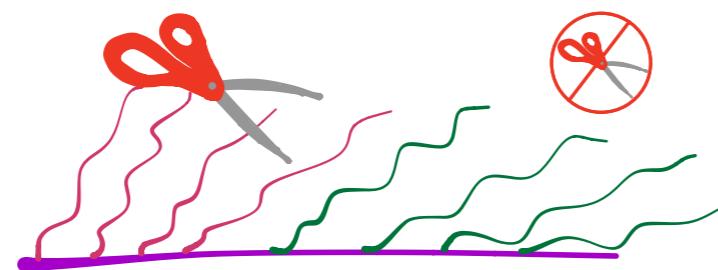
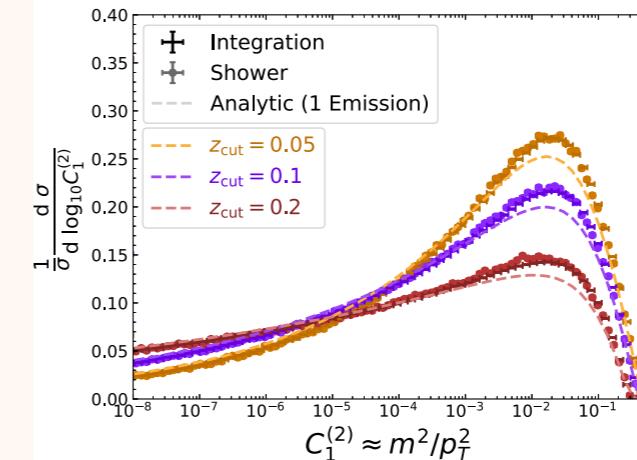
Recursive Safe Subtraction: tree-based approx. to optimal transport grooming

Fixed coupling, **multiple emission** calculations:

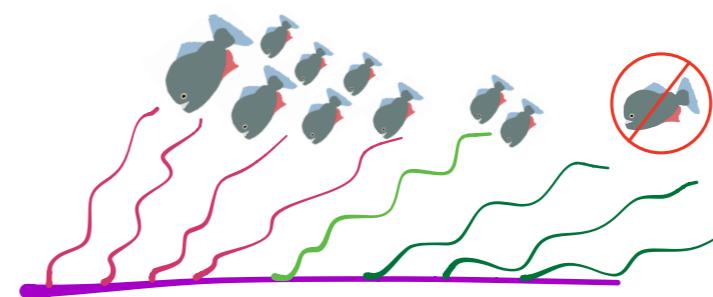
Soft Drop/mMDT



PIRANHA-RSS ($f = 1$)



Sharp cutoff → kink



No sharp cutoff → smooth

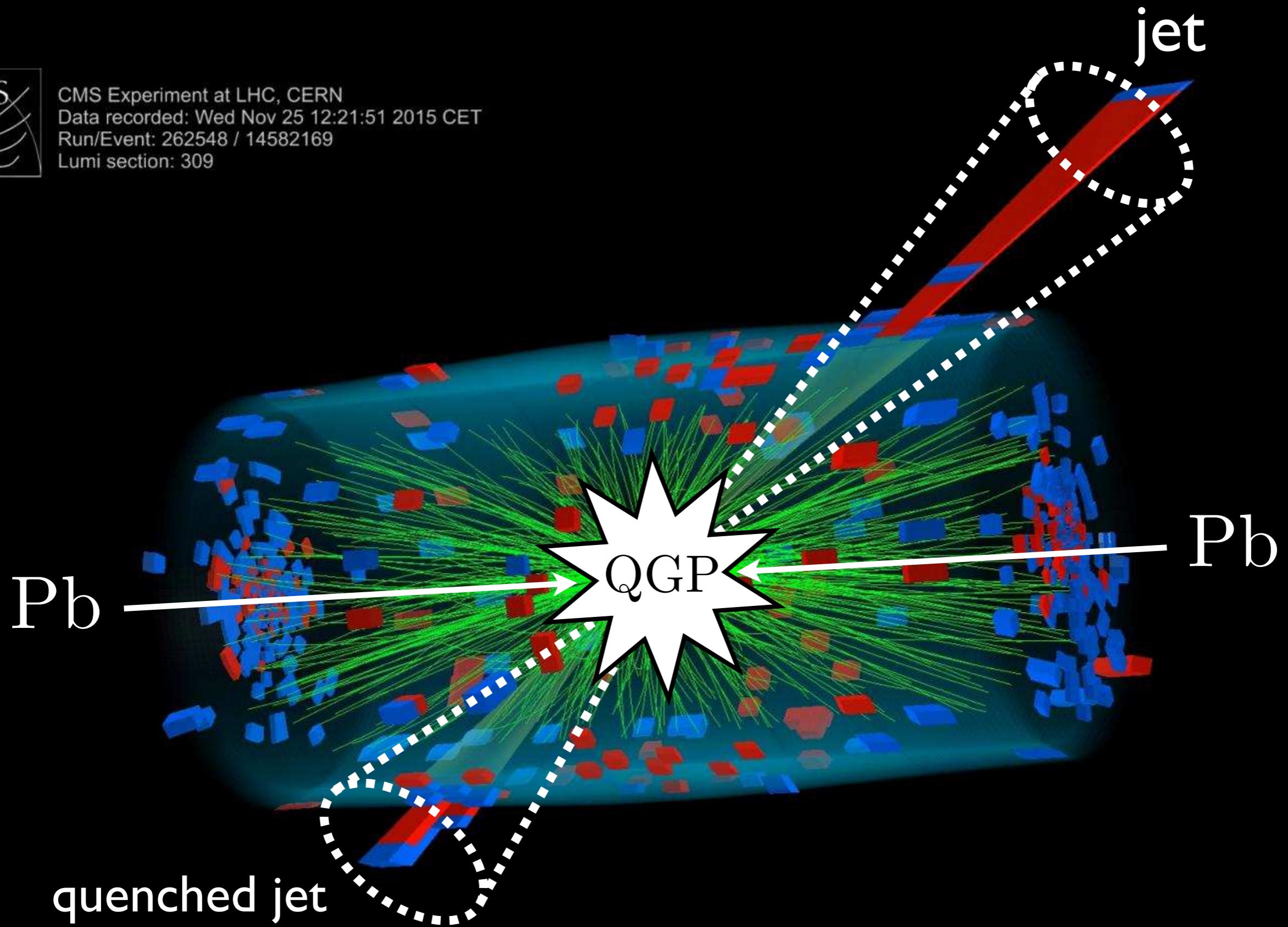
[Slides from Sam Alipour-fard]

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





CMS Experiment at LHC, CERN
Data recorded: Wed Nov 25 12:21:51 2015 CET
Run/Event: 262548 / 14582169
Lumi section: 309

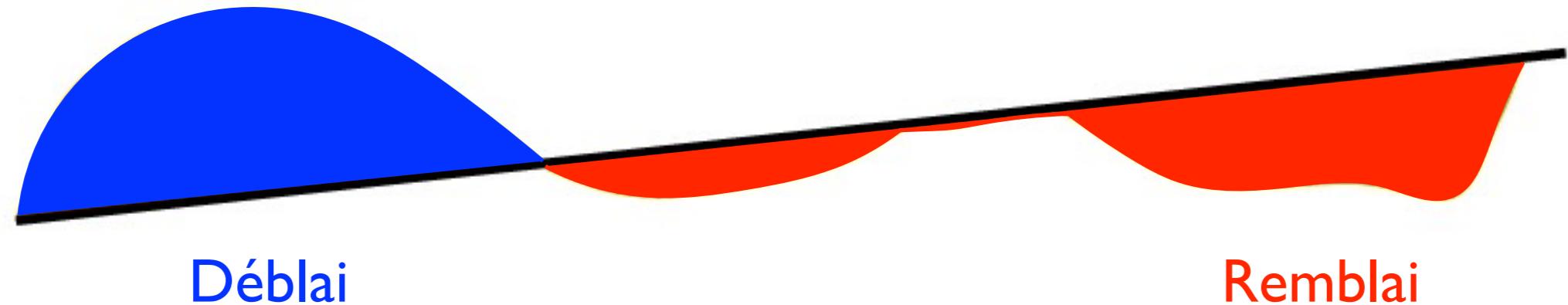
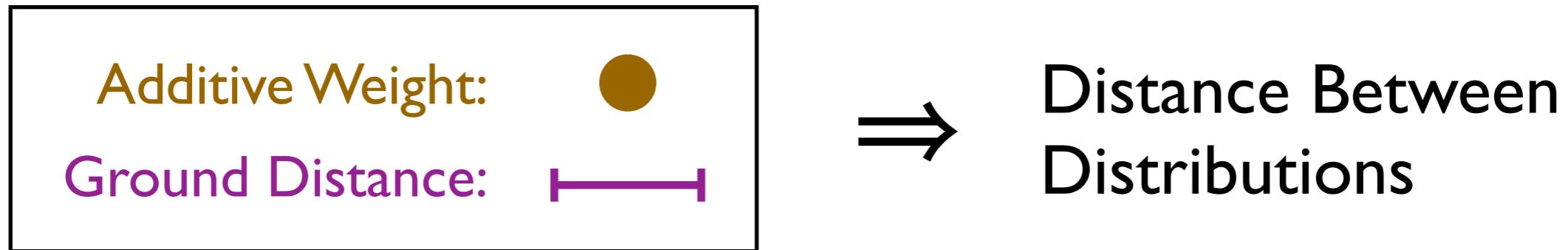


The Earth Mover's Distance

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](#)]

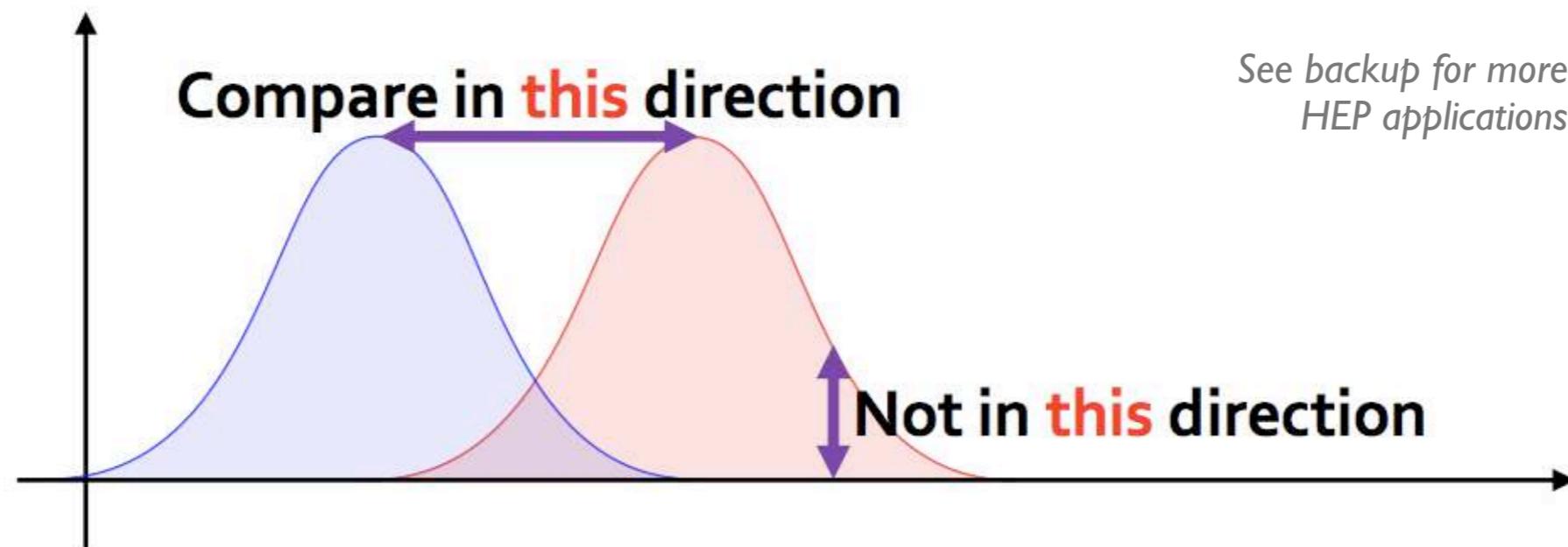
The Earth Mover's Distance

Optimal Transport:

[Peleg, Werman, Rom, [IEEE 1989](#);
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Pele, Werman, [ECCV 2008](#); Pele Taskar, [GSI 2013](#)]

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

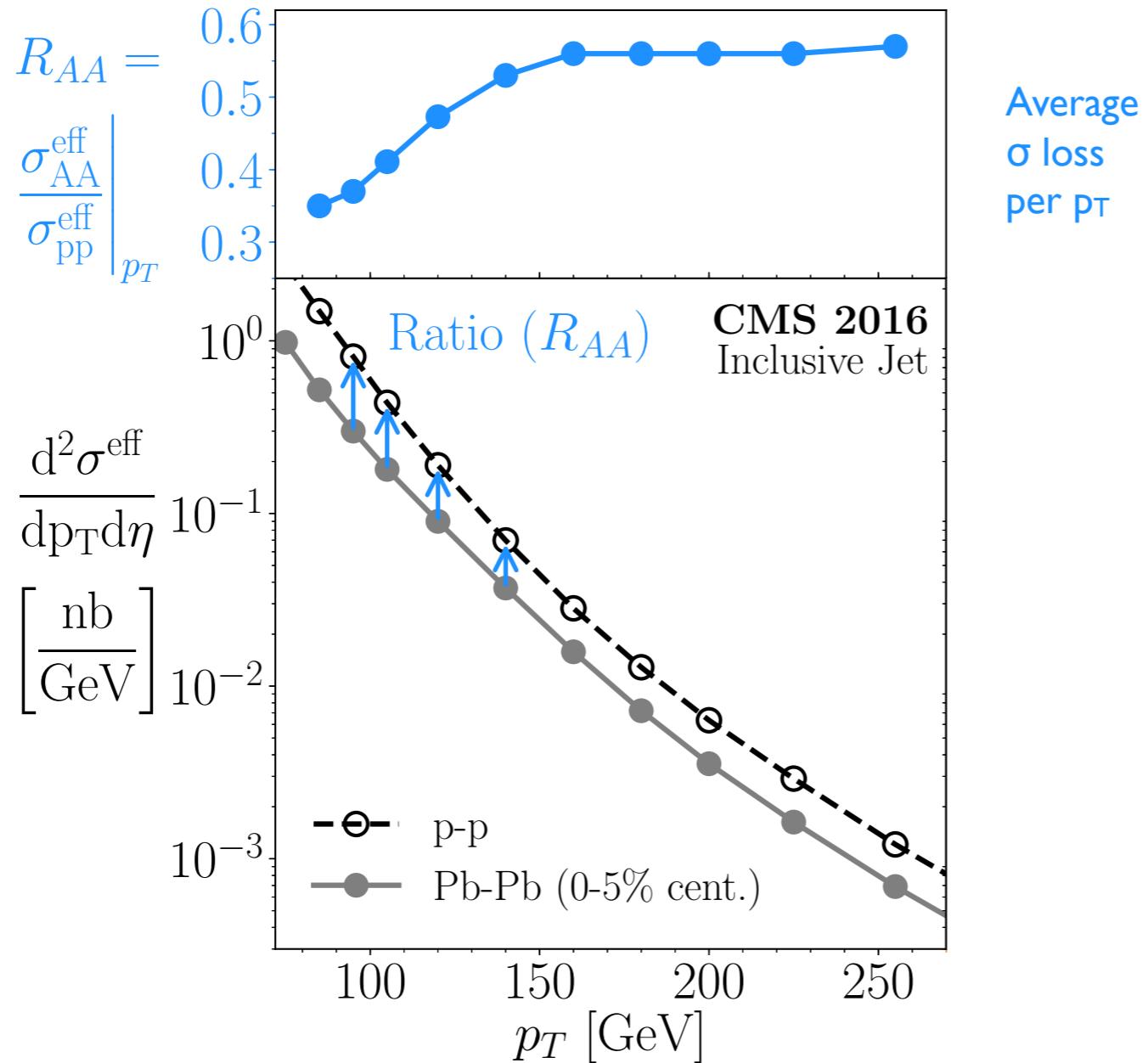
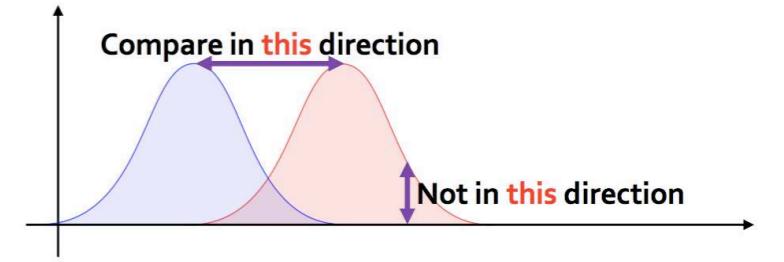
“Horizontal” comparison (EMD) yields better
dynamic range than “vertical” comparison (e.g. KL)



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

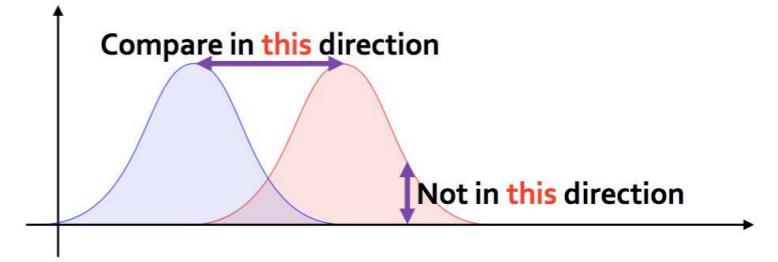
[h/t Niles-Weed, [ML4Jets 2020](#); Monge, 1781; Kantorovich, 1939; Vaserštejn, 1969; [Wikipedia](#)]

Jet Quenching via RAA?

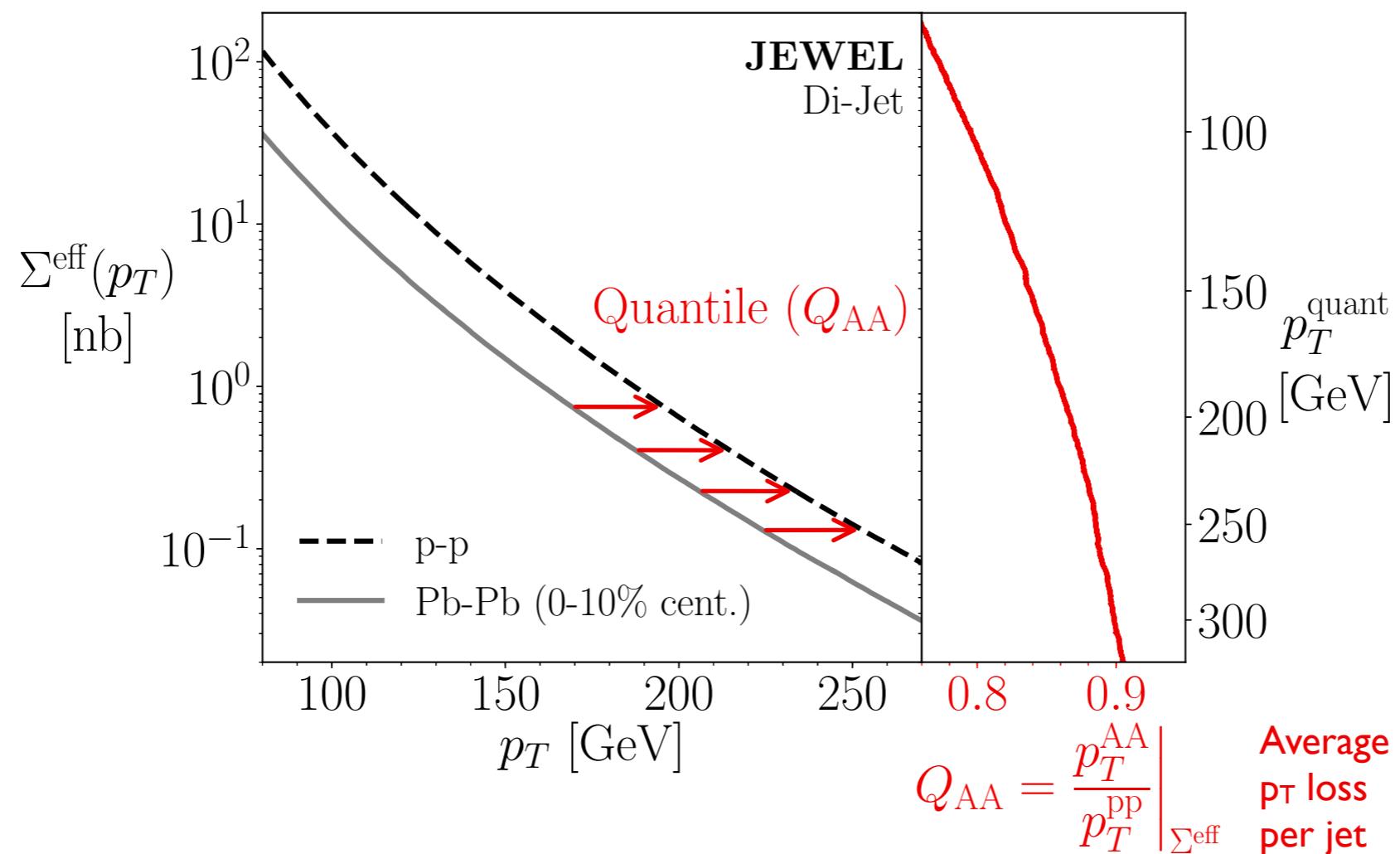


Jet Quenching via QAA!

Quantile matching as optimal transport



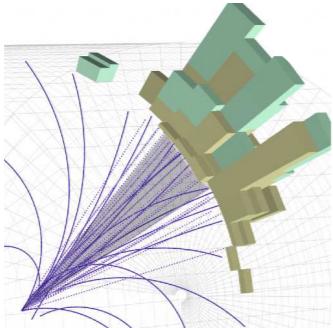
(For the record, we had no idea about OT when we suggested this method)



[Brewer, Milhano, JDT, PRL 2019]

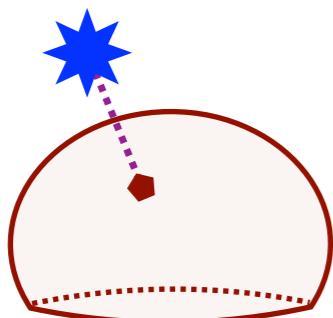


Optimal Transport for QCD and Jets



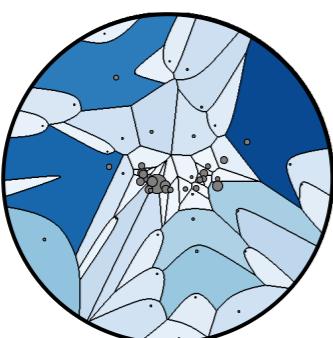
Going with the Flow

Restricting our attention to IRC safe information unlocks the power of optimal transport theory



Flowing into the Past

The energy mover's distance yields a new geometric language to understand old concepts/techniques in QCD and jets



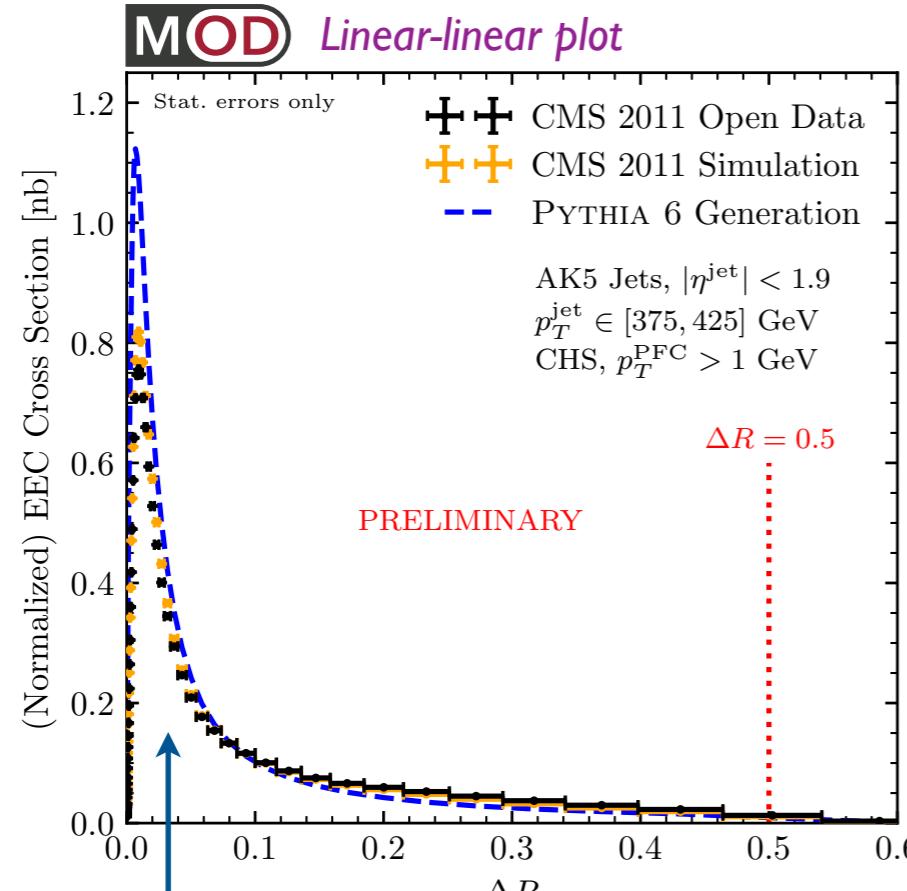
Flowing into the Future

Taking a machine learning / data science perspective could point the way to the next advances in particle/nuclear theory

Too Many Backup Slides

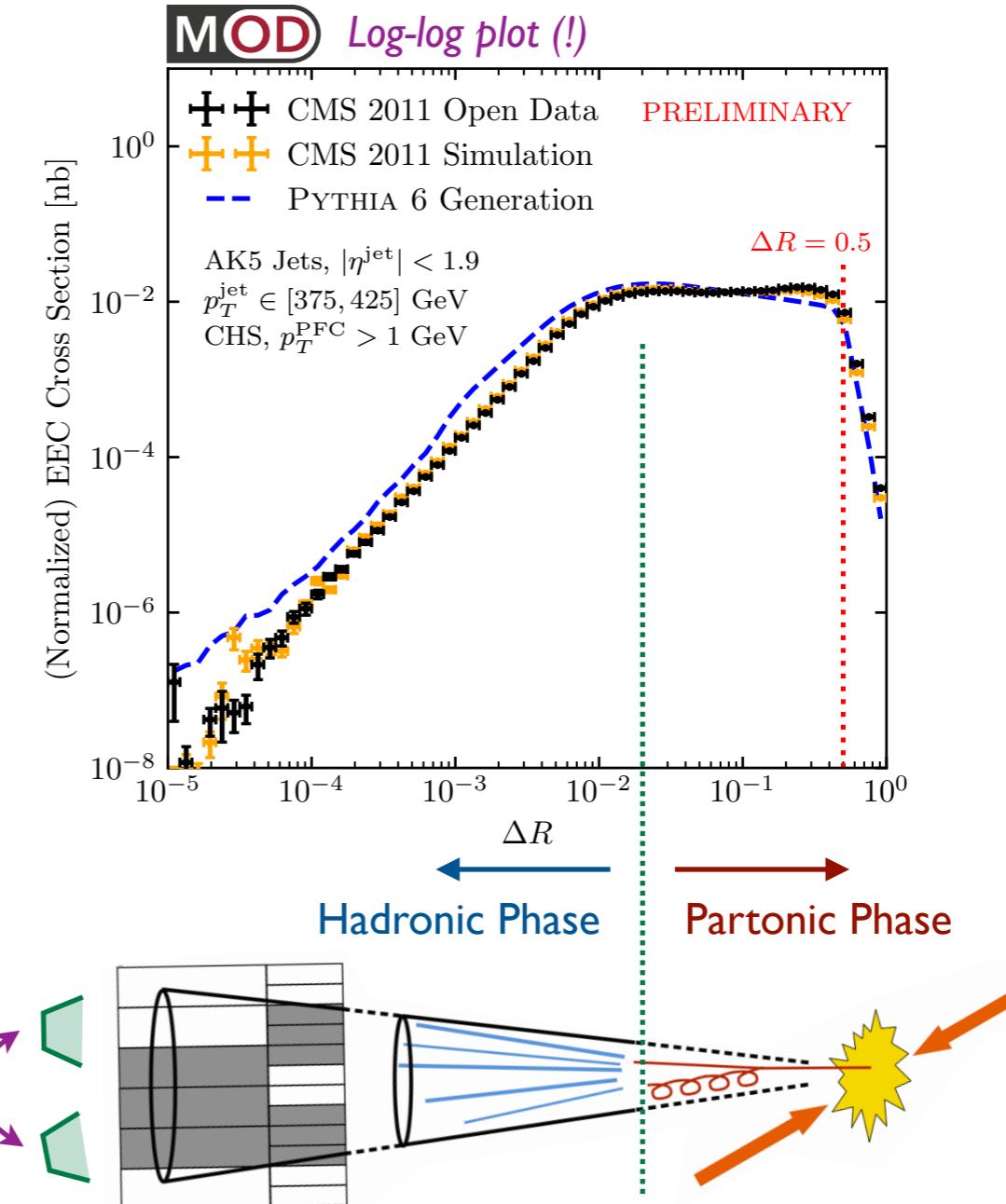
Stealing Ian's Thunder

QCD Phase Transition in Jets?



Are we learning something about small angle limit of QCD?

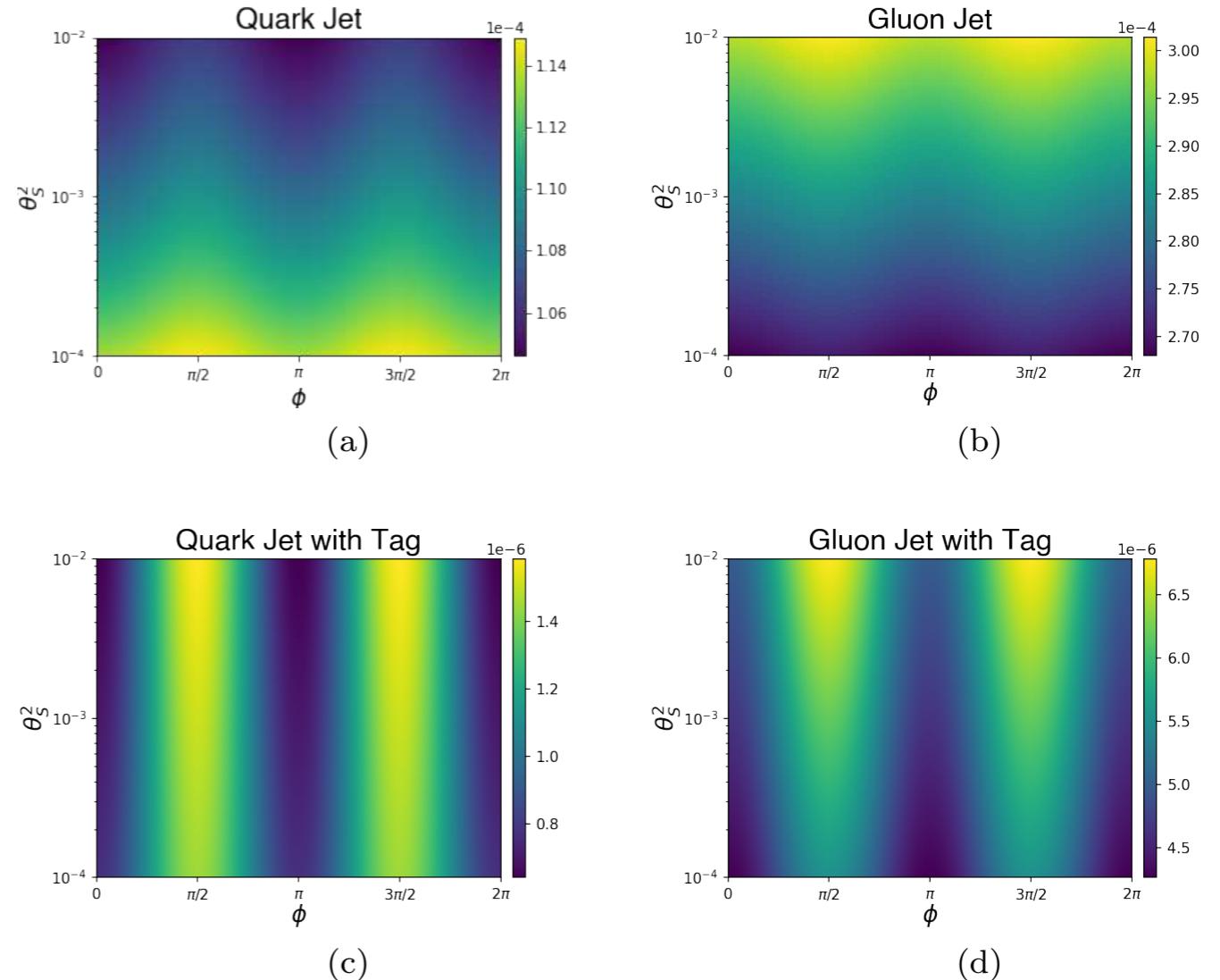
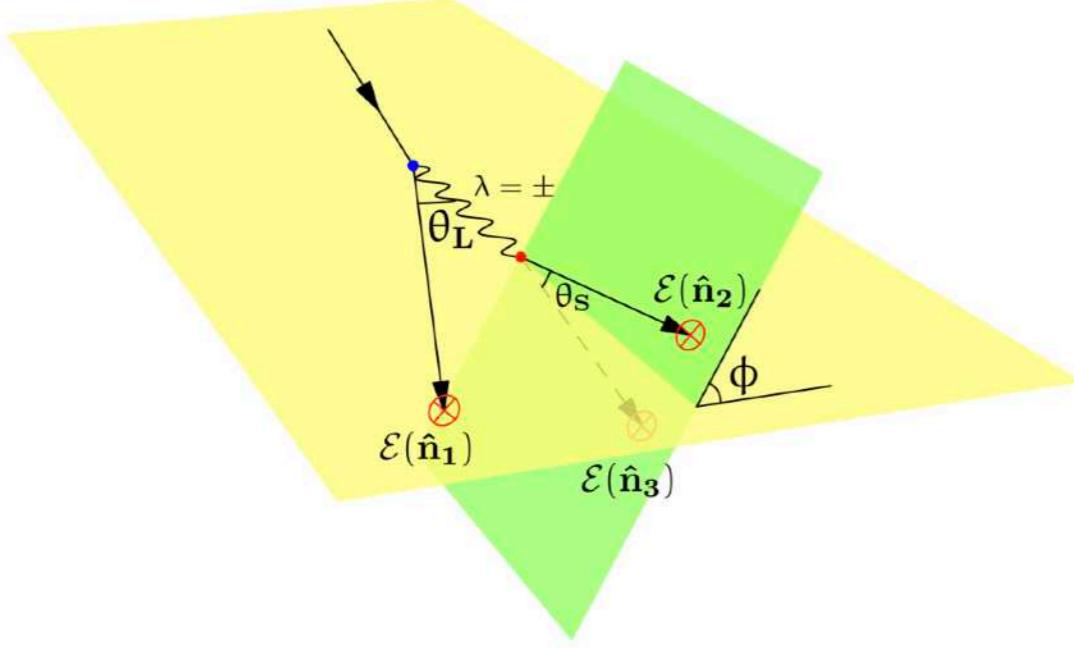
First Jet EEC Plot from the LHC (!)



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



Fun with Three Point Correlators



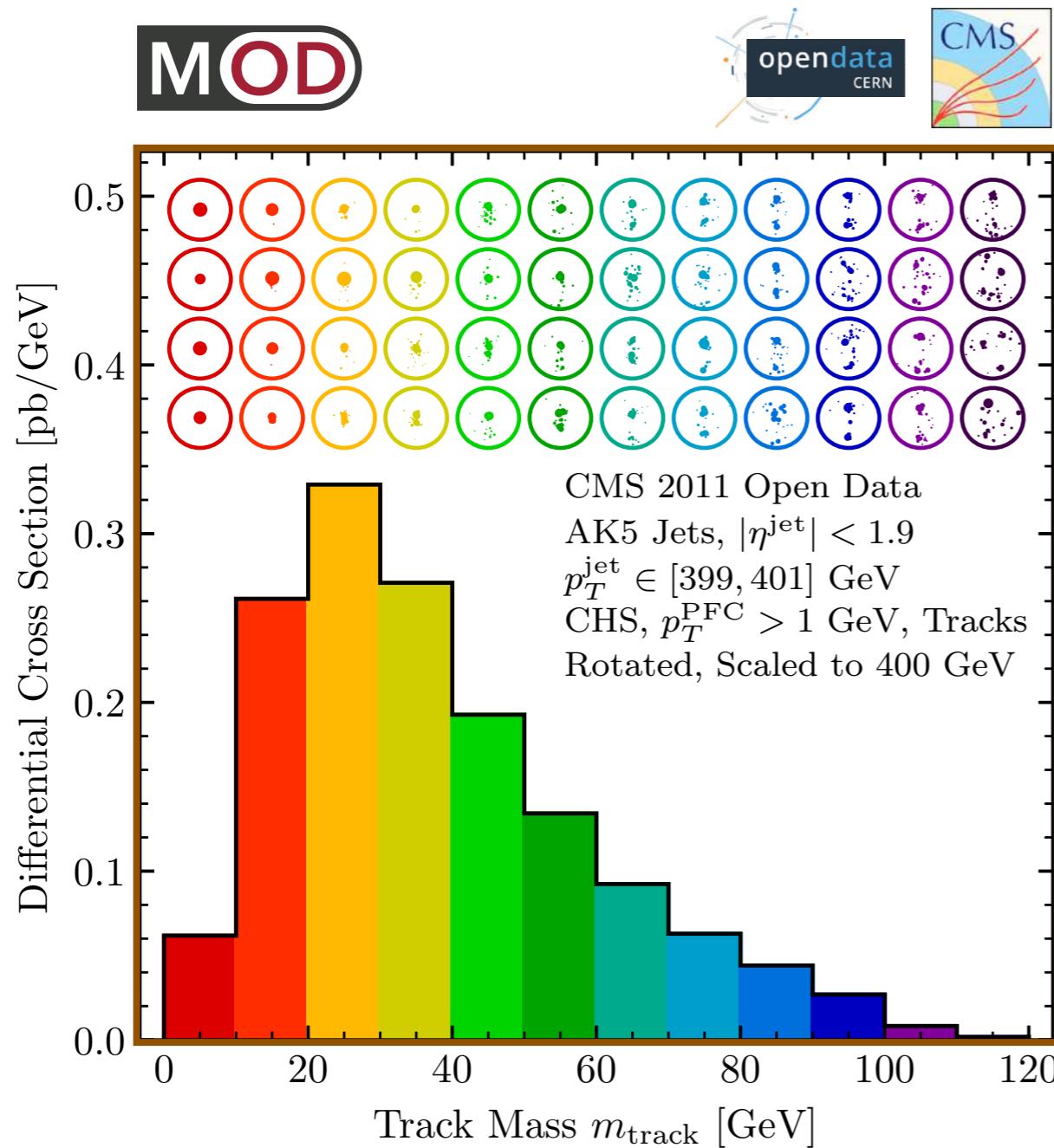
(with help from b-tagging)

Extracting quantum interference effects of spinning gluons!

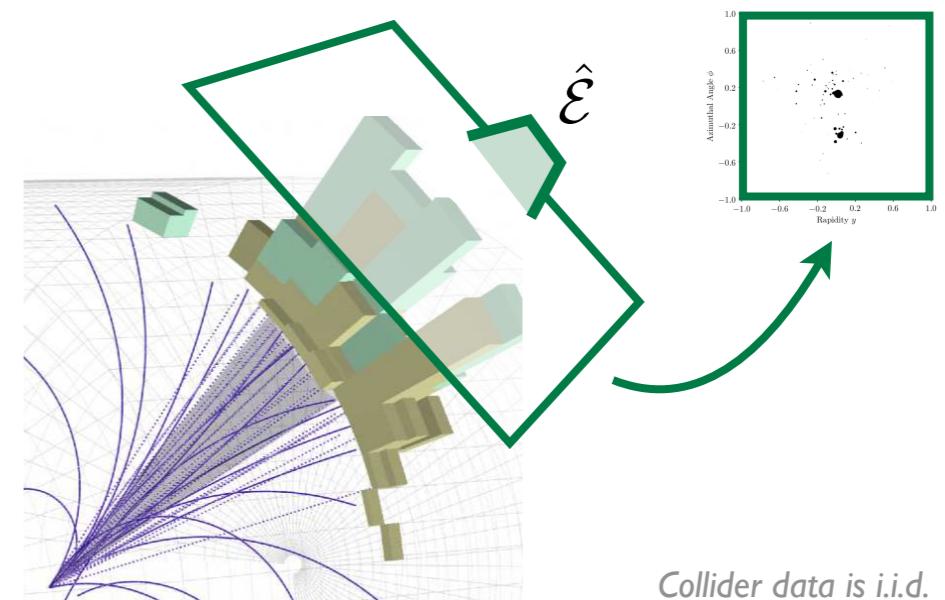
[Chen, Moult, Zhu, [PRL 2021](#)]

Plotting Paradigms

The Forest and the Trees



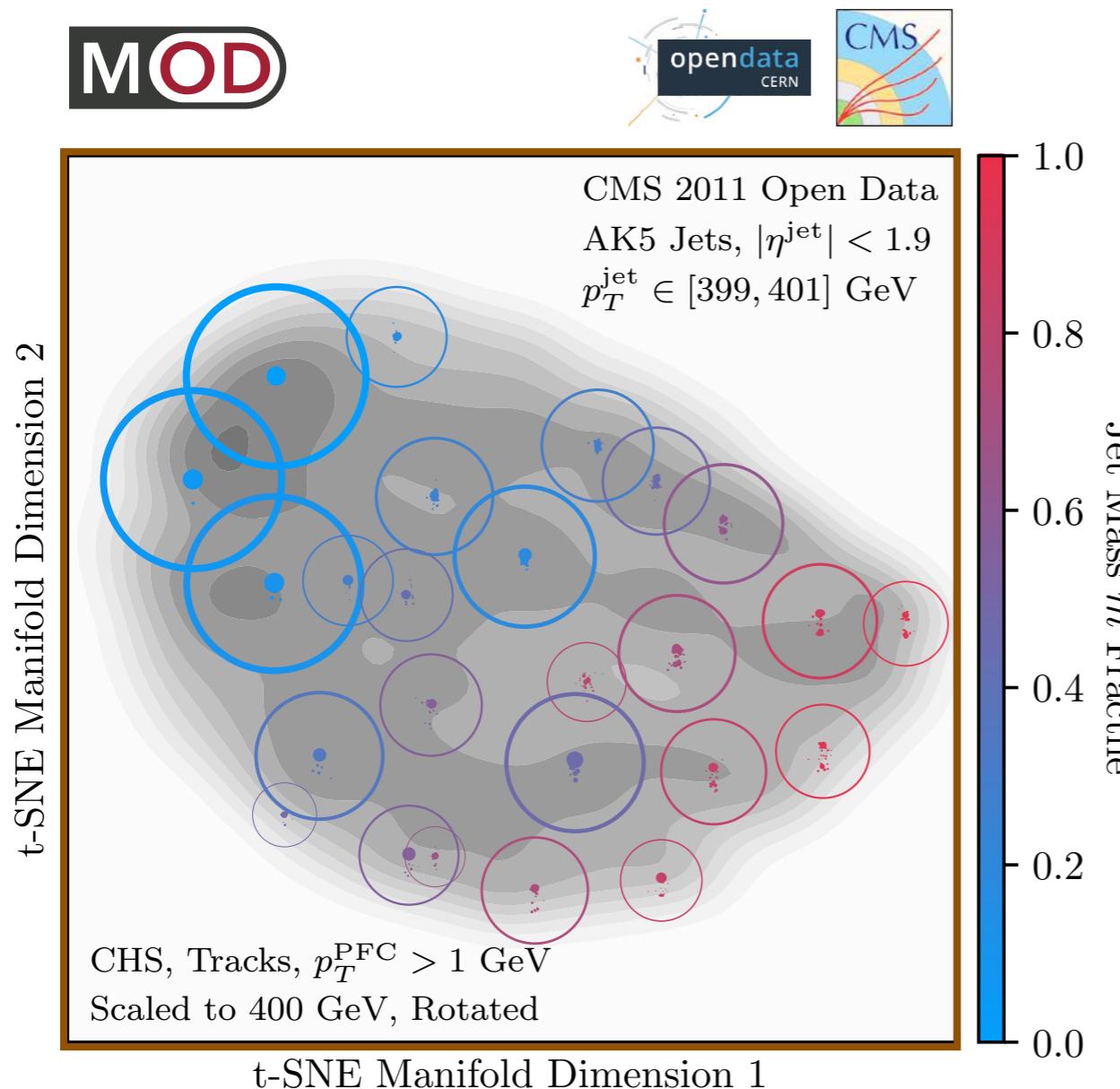
A *Histogram of Observables*



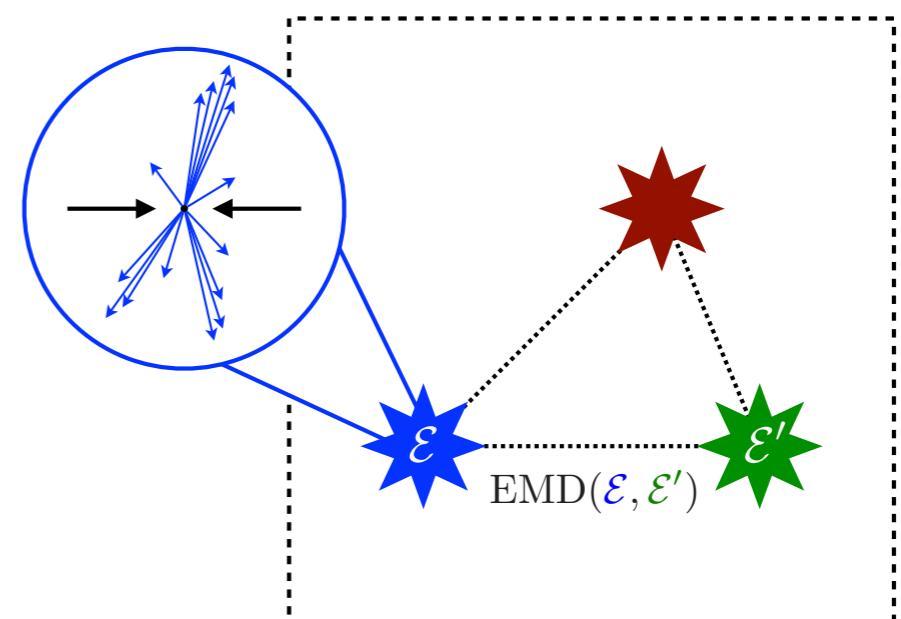
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;
using CMS Open Data]



Building the Forest from the Trees



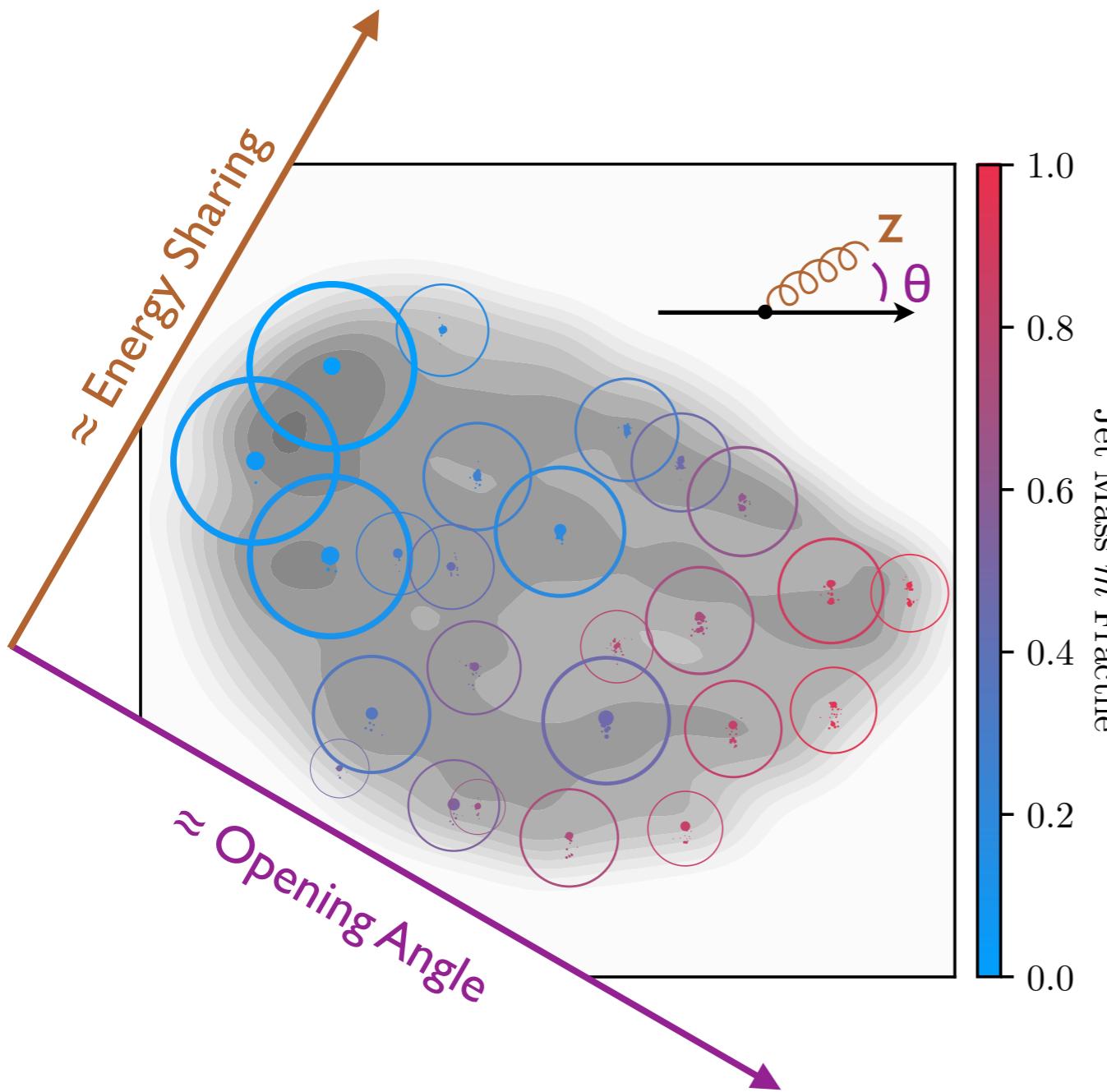
The Space of Energy Flows



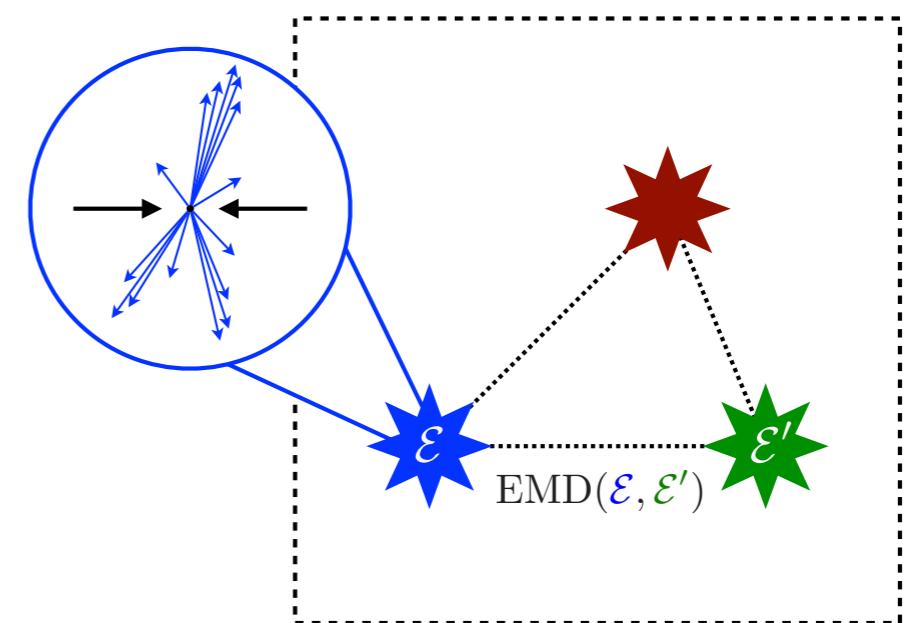
[Komiske, Mastandrea, Metodiev, Naik, JDT, [PRD 2020](#);
using van der Maaten, Hinton, [JMLR 2008](#); using [CMS Open Data](#)]



Building the Forest from the Trees



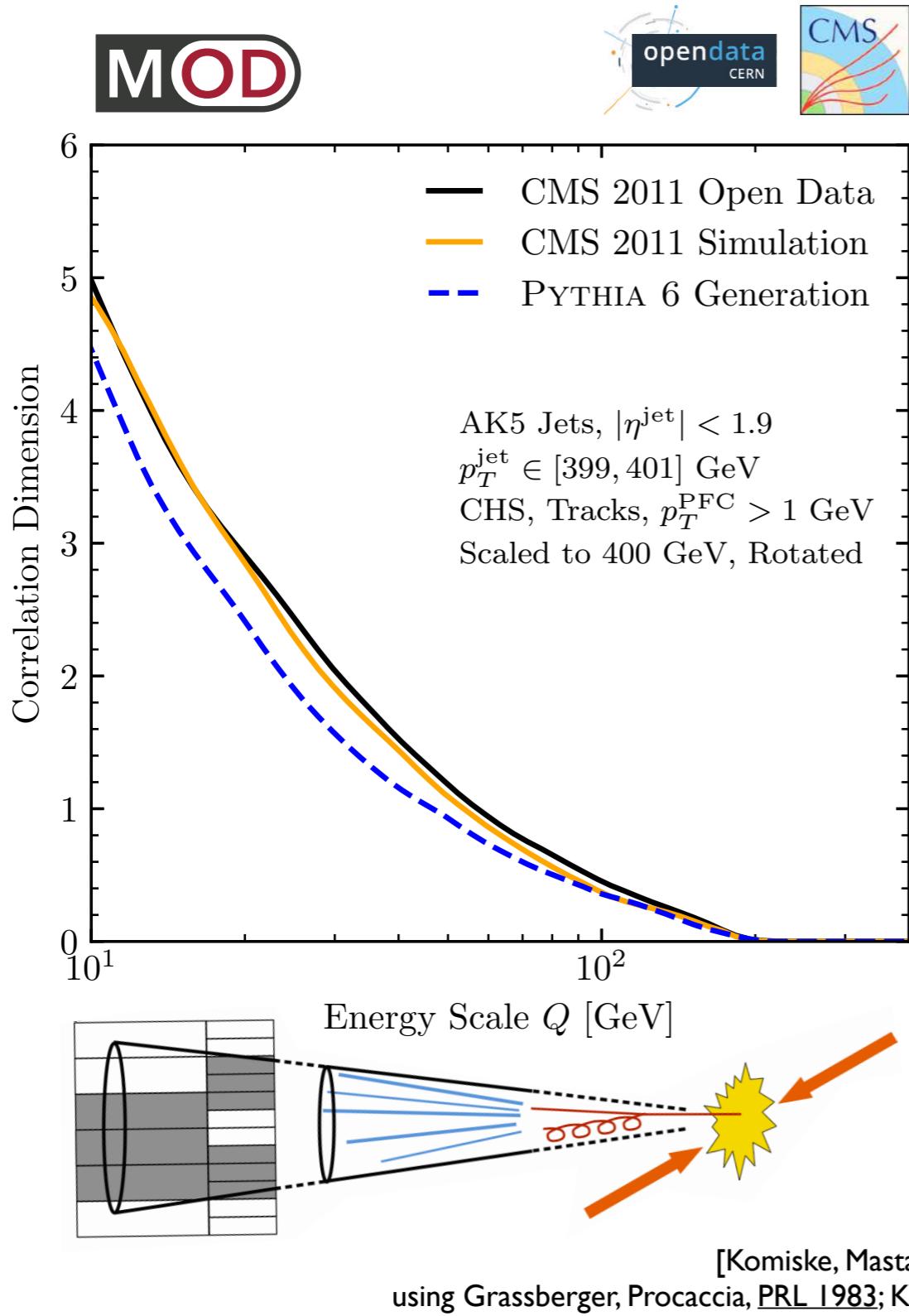
The Space of Energy Flows



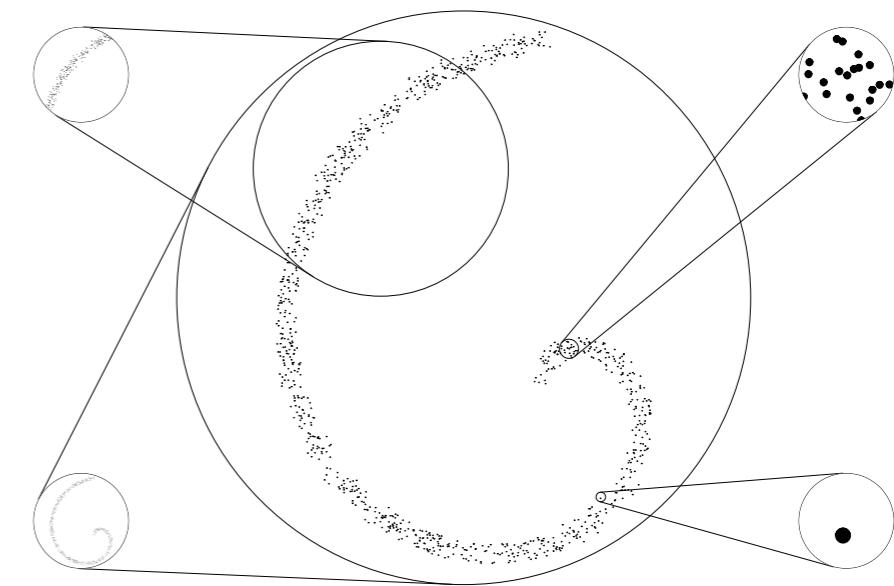
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;
using van der Maaten, Hinton, JMLR 2008; using CMS Open Data]



A Super-Fractal Forest made from Trees



Dimension of Space of Energy Flows

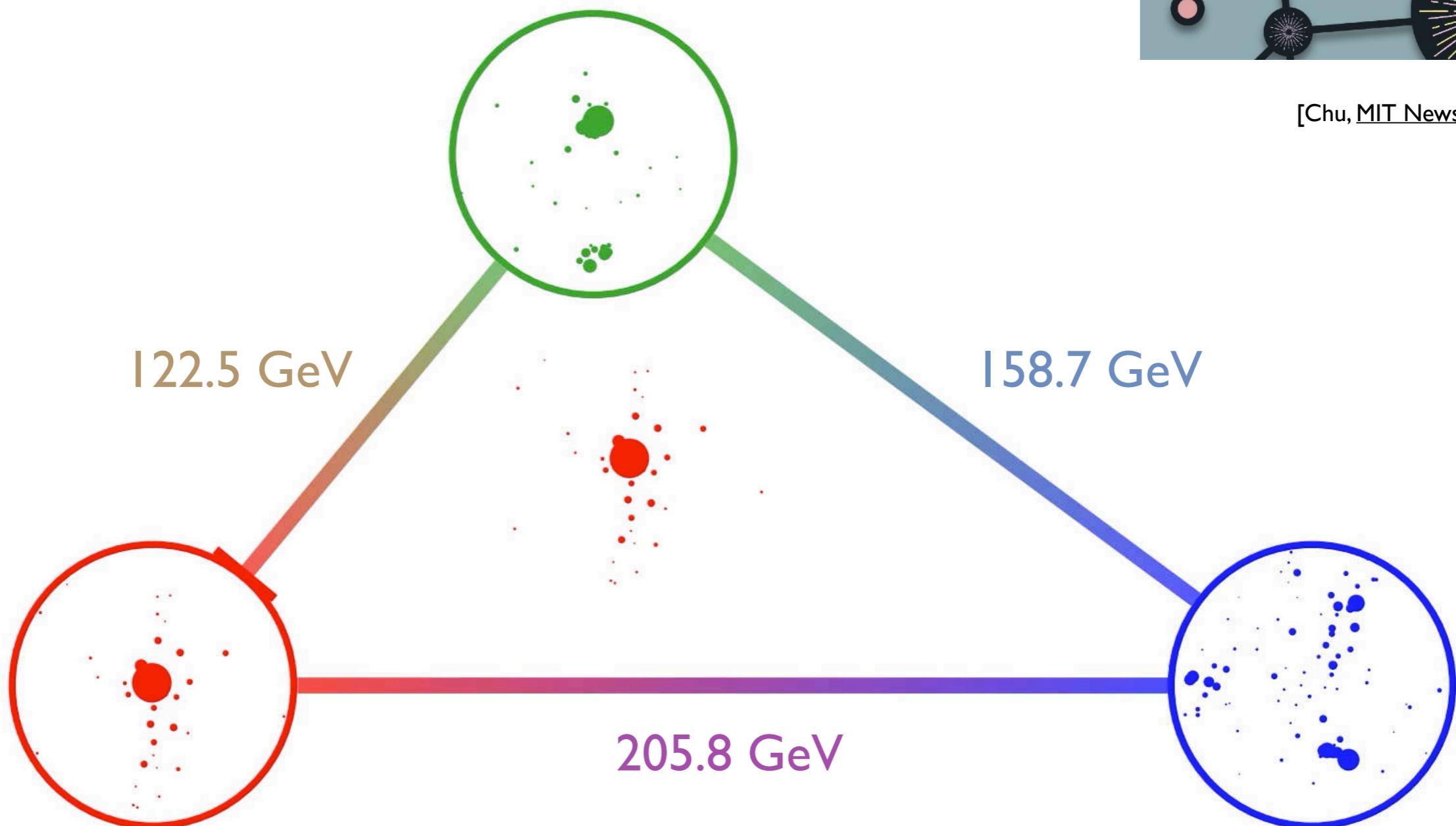


Movies that probably won't work

Similarity of Three Energy Flows



[Chu, MIT News July 2019]

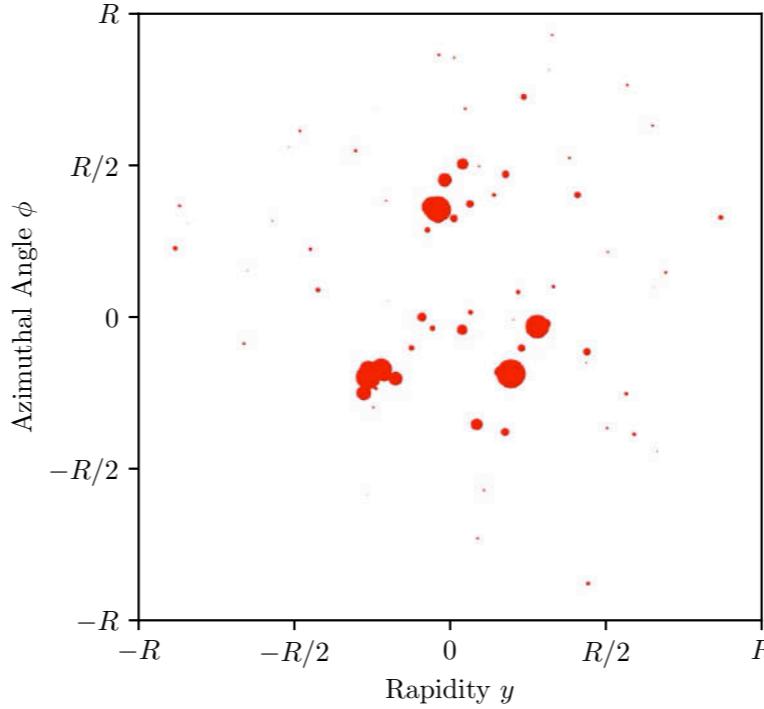


[Komiske, Metodiev, JDT, [PRL 2019](#); code at Komiske, Metodiev, JDT, [energyflow.network](#); see alternative graph network approach in Mullin, Pacey, Parker, White, Williams, [JHEP 2021](#)]

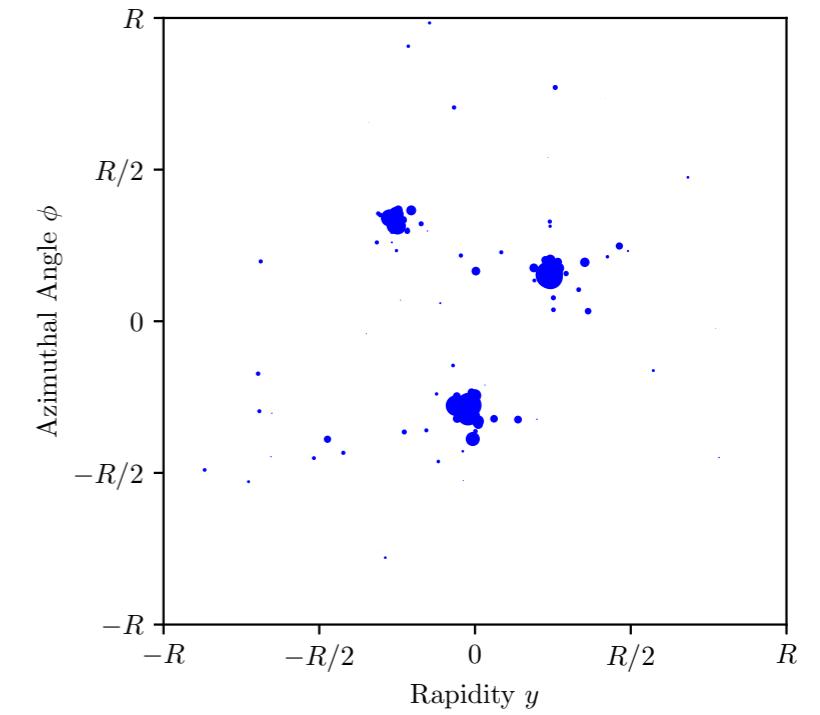
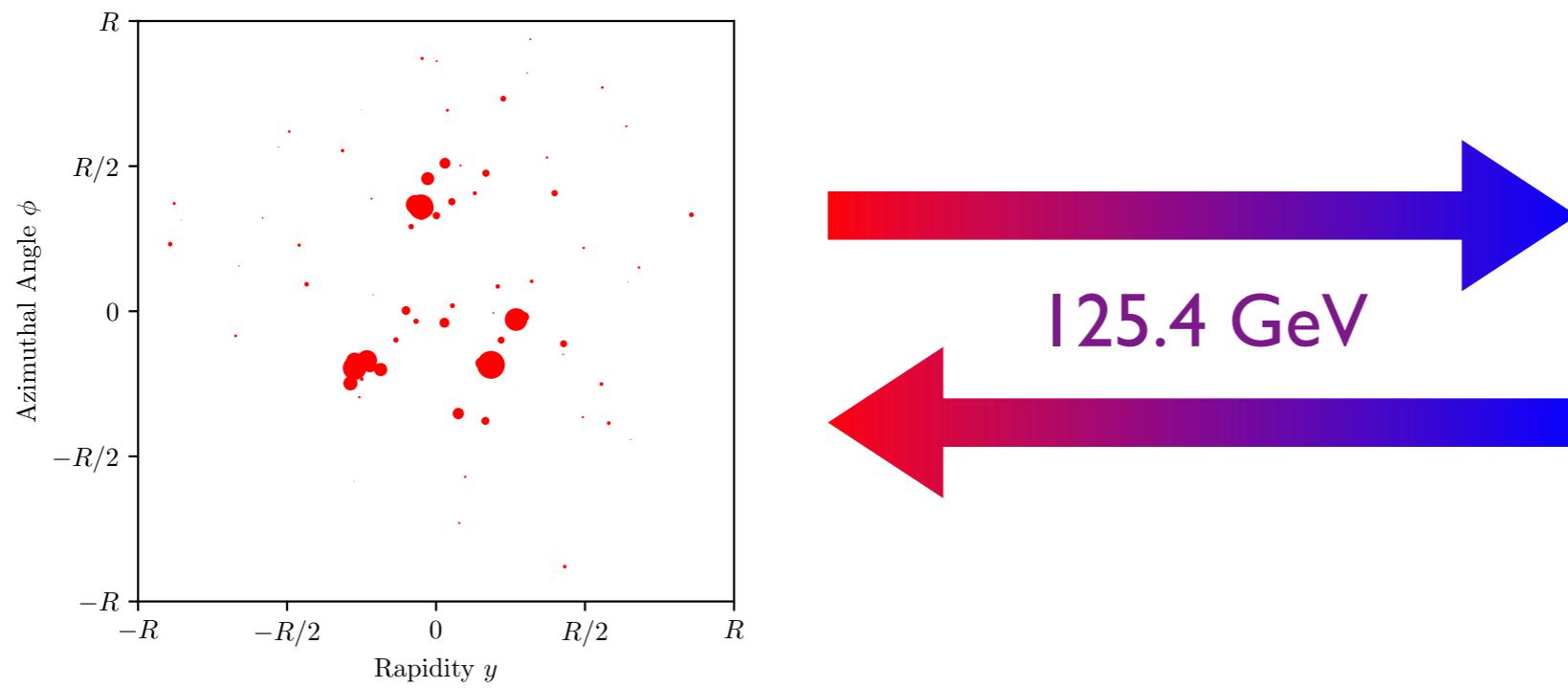


Similarity of Two Energy Flows

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



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



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

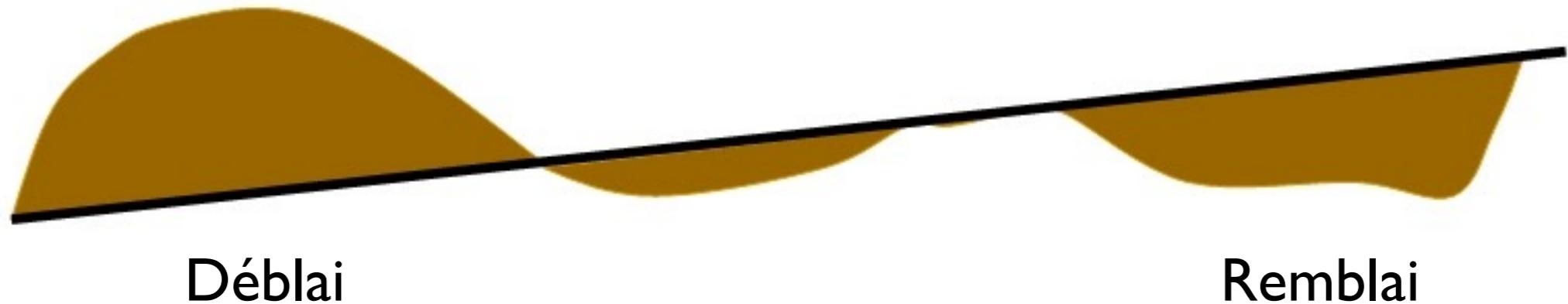
More About Optimal Transport

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](#)]

On my reading list...

Renormalization Group Flow as Optimal Transport

Jordan Cotler^{1,2,3} and Semon Rezchikov⁴

¹*Harvard Society of Fellows, Cambridge, MA 02138 USA*

²*Black Hole Initiative, Harvard University, Cambridge, MA 02138 USA*

³*Center for Fundamental Laws of Nature, Harvard University, Cambridge, MA 02138 USA*

⁴*Department of Mathematics, Harvard University, Cambridge, MA 02138 USA*

Abstract

We establish that Polchinski's equation for exact renormalization group flow is equivalent to the optimal transport gradient flow of a field-theoretic relative entropy. This provides a compelling information-theoretic formulation of the exact renormalization group, expressed in the language of optimal transport. A striking consequence is that a regularization of the relative entropy is in fact an RG monotone. We compute this monotone in several examples. Our results apply more broadly to other exact renormalization group flow equations, including widely used specializations of Wegner-Morris flow. Moreover, our optimal transport framework for RG allows us to reformulate RG flow as a variational problem. This enables new numerical techniques and establishes a systematic connection between neural network methods and RG flows of conventional field theories.

[Cotler, Rezchikov, [arXiv 2022](#)]

More QCD Slides

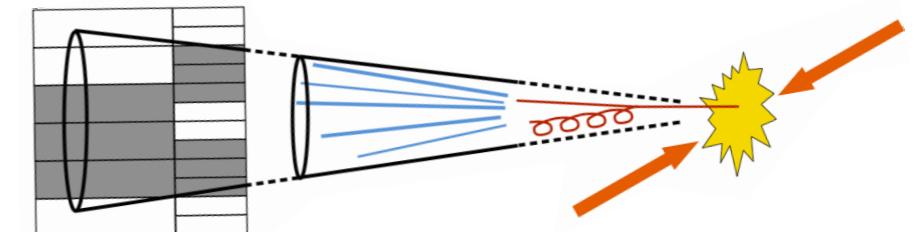
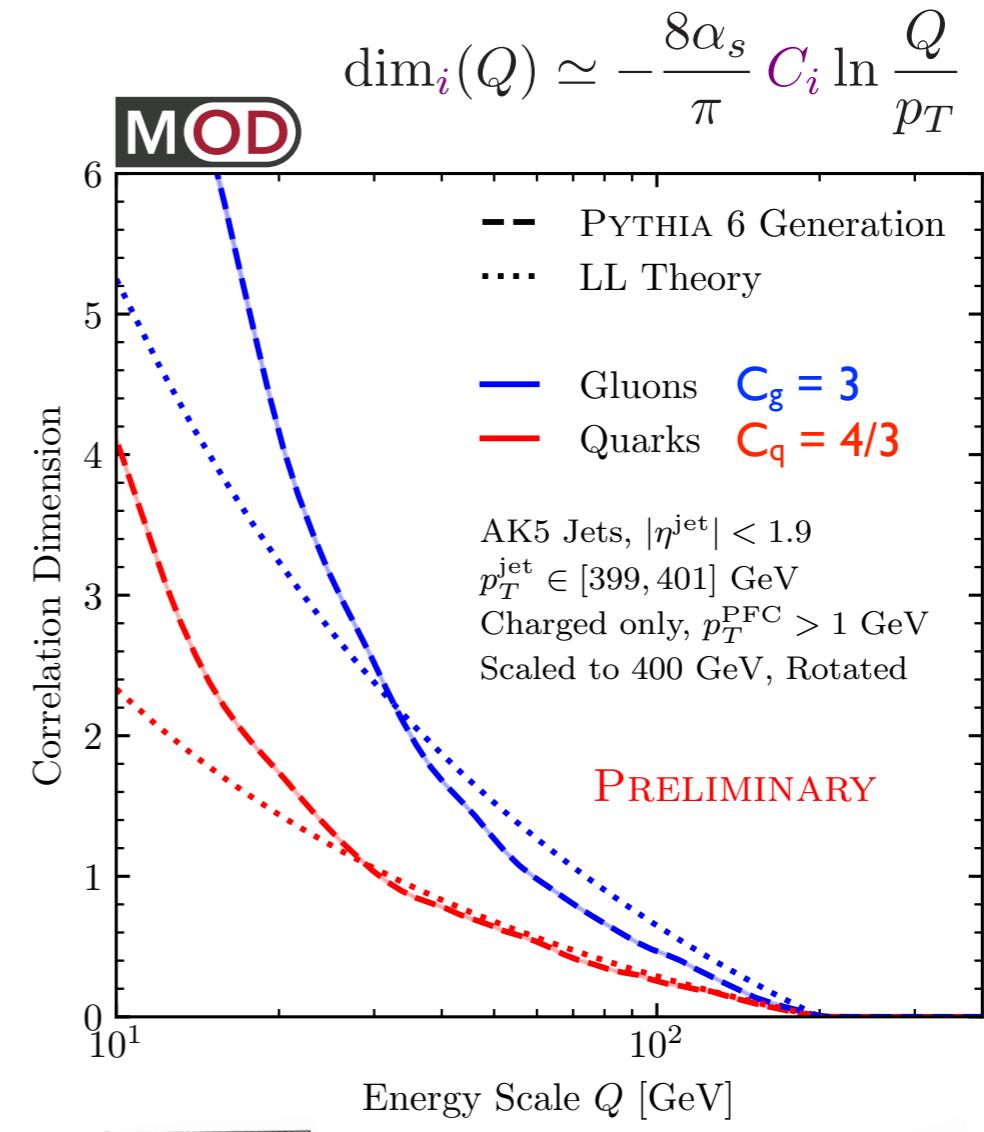
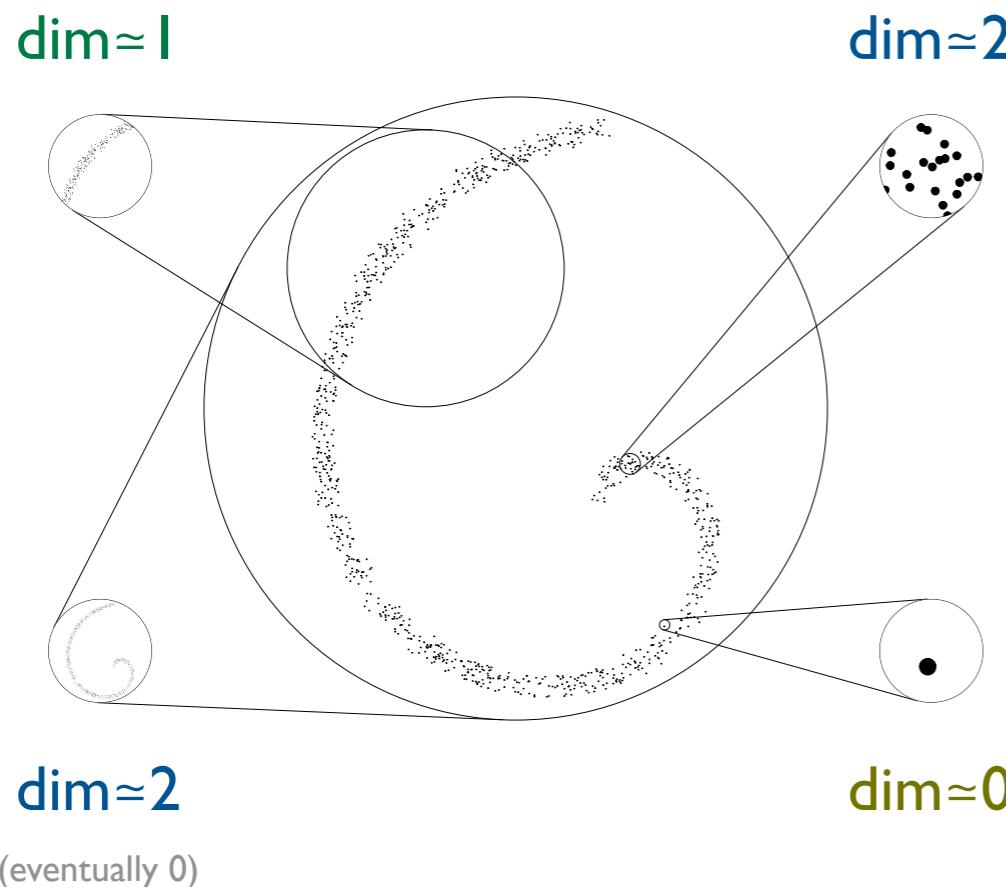
Dimensionality of Space of Jets



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

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

[Grassberger, Procaccia, [PRL 1983](#); Kégl, [NIPS 2002](#)]



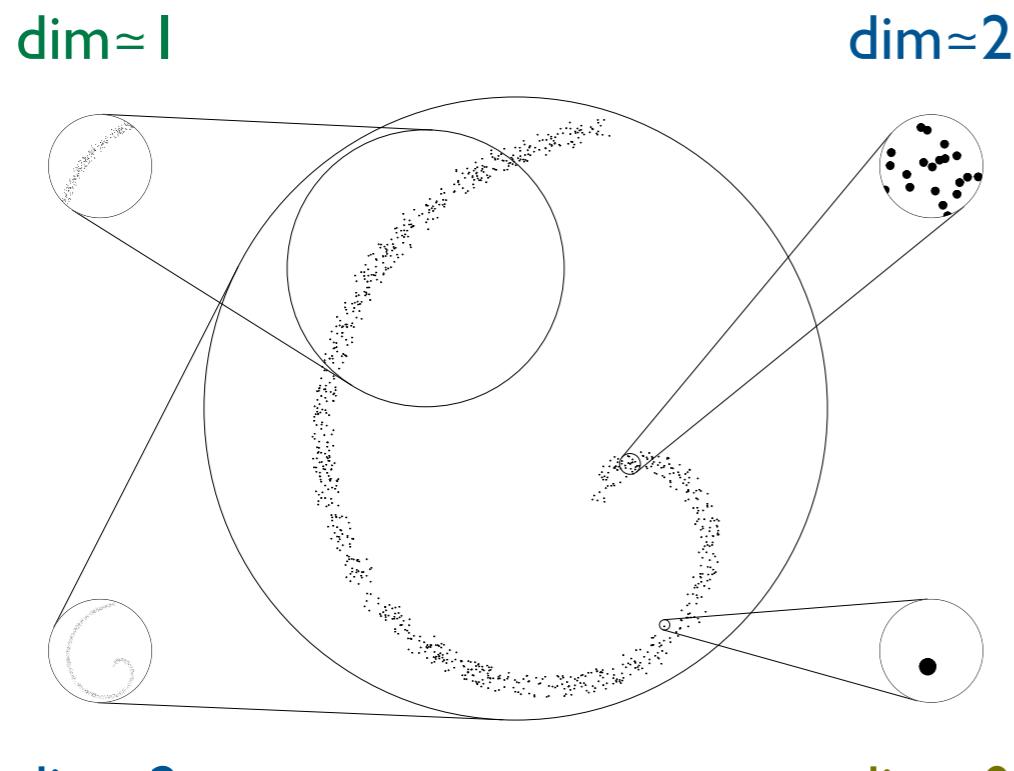
Dimensionality of Space of Jets



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

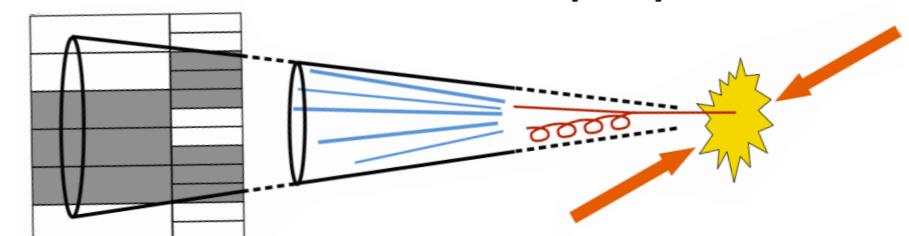
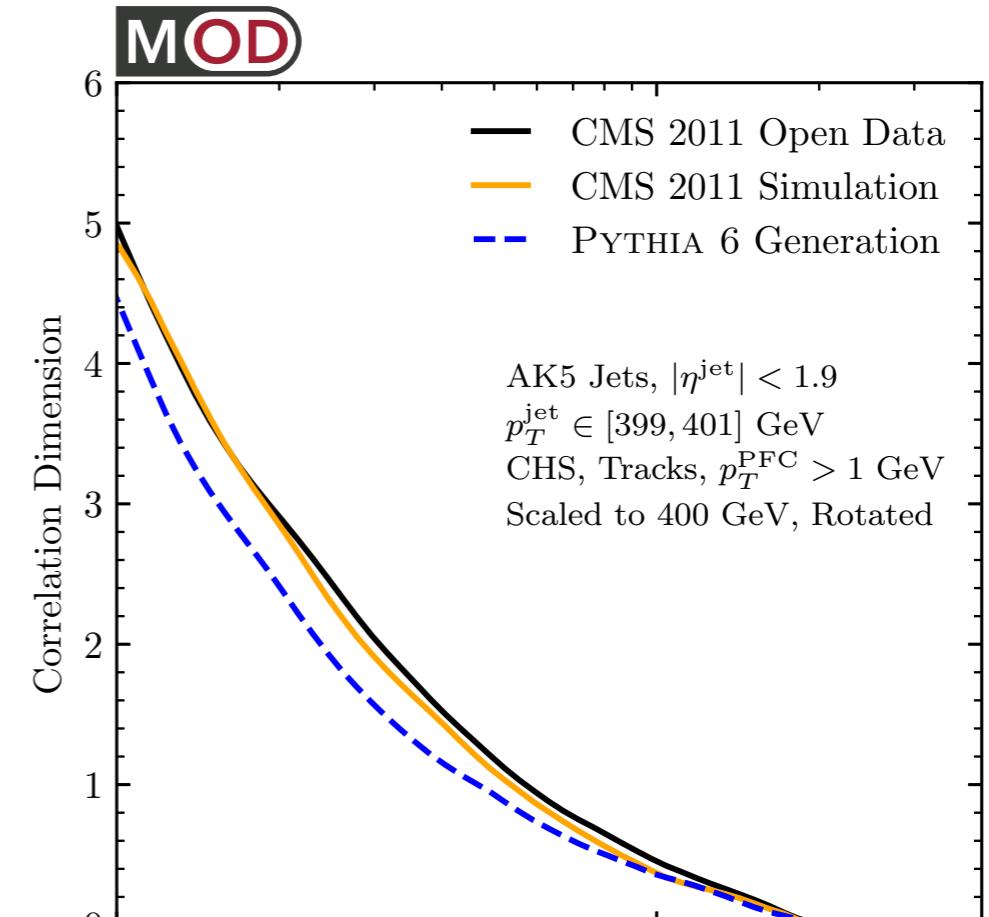
$$\Rightarrow \dim(r) \sim r \frac{\partial}{\partial r} \ln N_{\text{neighbors}}(r)$$

[Grassberger, Procaccia, [PRL 1983](#); Kégl, [NIPS 2002](#)]



(eventually 0)

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



The Spectrum of Safety

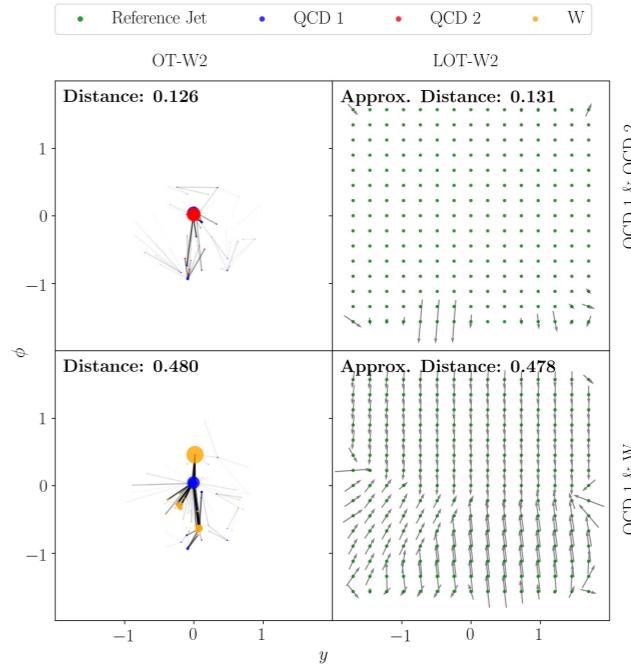
All Observables	Comments
Multiplicity ($\sum_i 1$)	IR unsafe and C unsafe
Momentum Dispersion [65] ($\sum_i E_i^2$)	IR safe but C unsafe
Sphericity Tensor [66] ($\sum_i p_i^\mu p_i^\nu$)	IR safe but C unsafe
Number of Non-Zero Calorimeter Deposits	C safe but IR unsafe
Defined on Energy Flows	
Pseudo-Multiplicity ($\min\{N \mid \mathcal{T}_N = 0\}$)	Robust to exact IR or C emissions
Infrared & Collinear Safe	
Jet Energy ($\sum_i E_i$)	Disc. at jet boundary
Heavy Jet Mass [67]	Disc. at hemisphere boundary
Soft-Dropped Jet Mass [38, 68]	Disc. at grooming threshold
Calorimeter Activity [69] (N_{95})	Disc. at cell boundary
Sudakov Safe	
Groomed Momentum Fraction [39] (z_g)	Disc. on 1-particle manifold
Jet Angularity Ratios [37]	Disc. on 1-particle manifold
N -subjettiness Ratios [47, 48] (τ_{N+1}/τ_N)	Disc. on N -particle manifold
V parameter [36] (Eq. (2.11))	Hölder disc. on 3-particle manifold
EMD Hölder Continuous Everywhere	
Thrust [40, 41]	
Spherocity [42]	
Angularities [70]	
N -jettiness [44] (\mathcal{T}_N)	
C parameter [71–74]	Resummation beneficial at $C = \frac{3}{4}$
Linear Sphericity [72] ($\sum_i E_i n_i^\mu n_i^\nu$)	
Energy Correlators [36, 75–77]	
Energy Flow Polynomials [15, 17]	

Alternative Measures

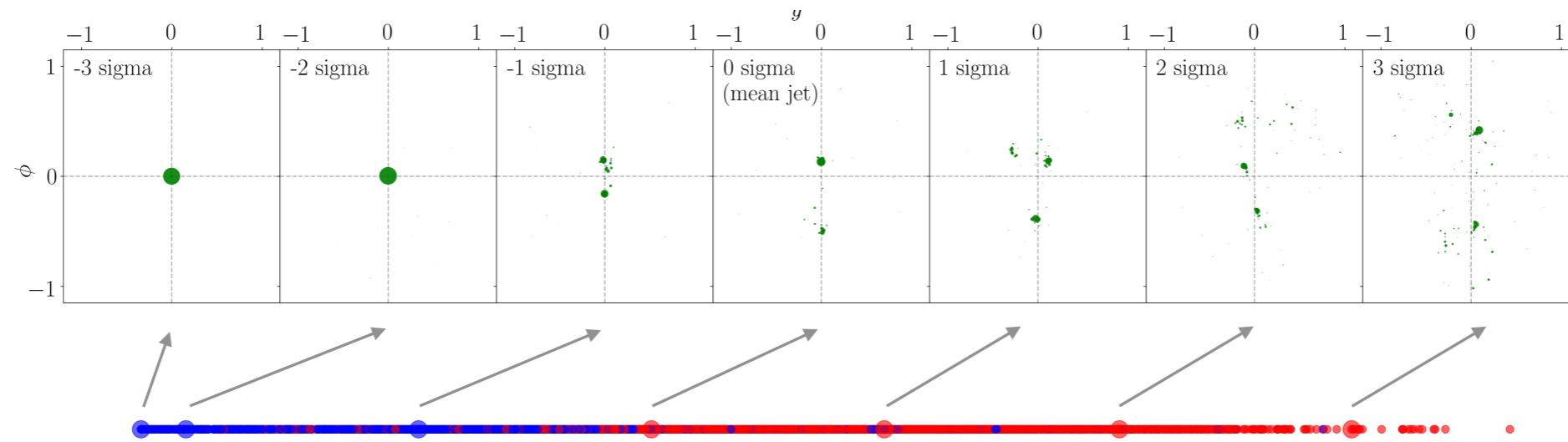
Linearized Optimal Transport

With the help of a reference event, transportation distances* can be efficiently mapped to Euclidean distances

* assuming the 2-Wasserstein measure



Enables coordinate-based techniques like Linear Discriminate Analysis

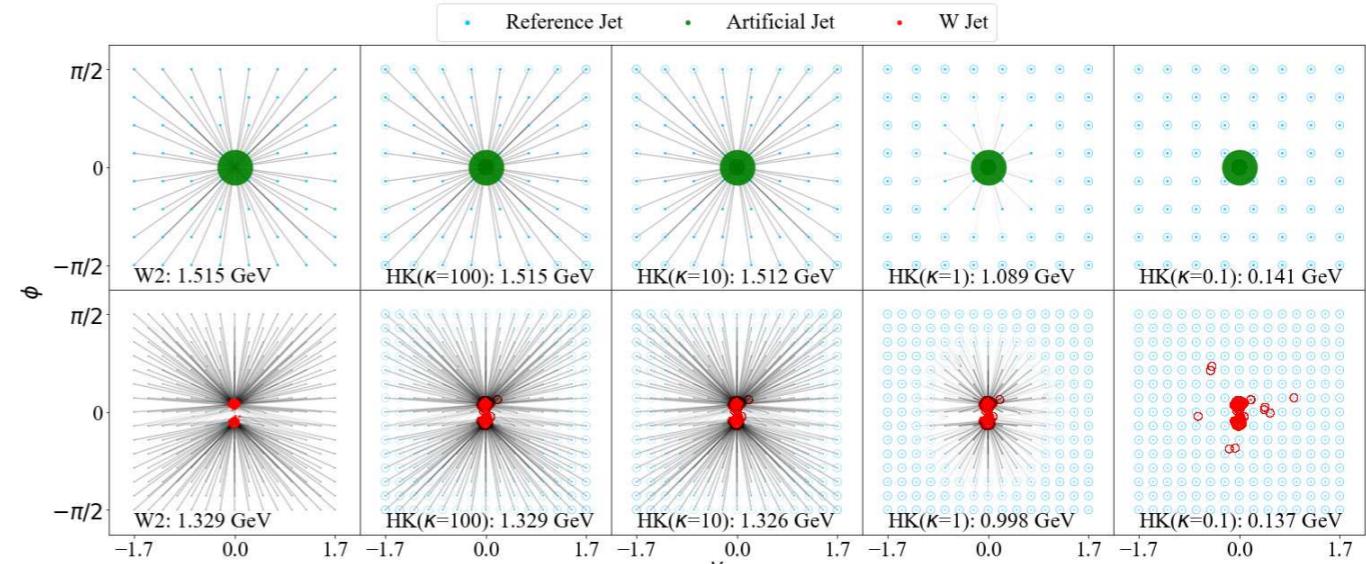


[Cai, Cheng, Craig, Craig, PRD 2020]

Opening a Dialogue Between Communities

HEP domain knowledge \Leftrightarrow interdisciplinary insights

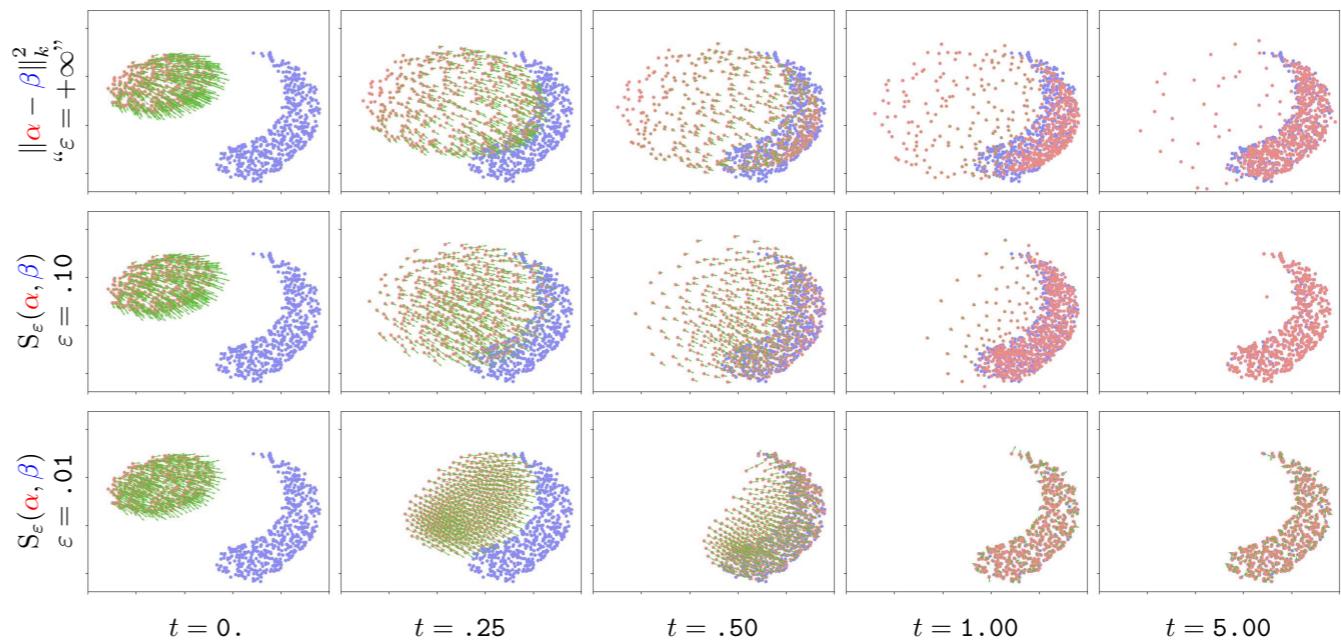
Analyzing Jets with
Linearized Transport
& Partial Transport



[Cai, Cheng, Craig, Craig, PRD 2020, arXiv 2021]

Interpolating between
Optimal Transport
& Kernel Methods

(see next slide to justify color coding)



[Feydy, Séjourné, Vialard, Amari, Trouvé, Peyré, arXiv 2018]

Siloing in the Scientific Community

$$\begin{aligned}\text{Kernel}_k(\alpha, \beta) &= \frac{1}{2} \langle \alpha, k \star \alpha \rangle - \langle \alpha, k \star \beta \rangle + \frac{1}{2} \langle \beta, k \star \beta \rangle \\ &= \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j k(x_i, x_j) - \sum_{i=1}^N \sum_{j=1}^M \alpha_i \beta_j k(x_i, y_j) + \frac{1}{2} \sum_{i=1}^M \sum_{j=1}^M \beta_i \beta_j k(y_i, y_j)\end{aligned}$$

Kernel methods. Formulas in the mould of Eqs. (3.99-3.101) are **ubiquitous in applied sciences**: from physics to machine learning, applying a convolution is the simplest way of modelling spatial correlations and pair-wise interactions. Unfortunately though, few papers and textbooks take the time to draw explicit links between fields that have, at first glance, very little in common. Before going any further, we devote a few pages to a short panorama around the six major interpretations of Eq. (3.99). As we identify with each other the theories of:

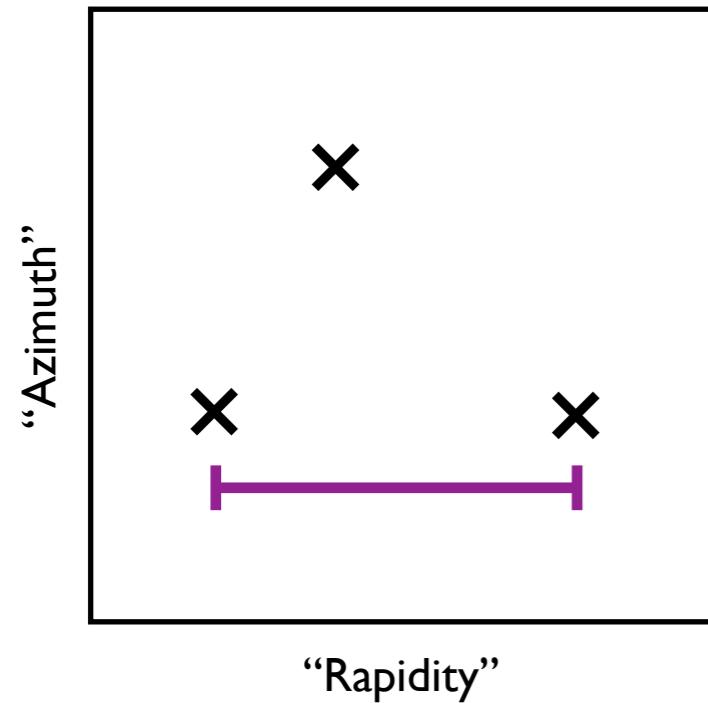
1. **Newtonian gravitation and electrostatics** in physics,
2. **blurred squared distances** in imaging sciences,
3. **Sobolev norms** in functional analysis,
4. **maximum mean discrepancies** in statistics,
5. **reproducing kernel Hilbert spaces** in machine learning and
6. **Kriging, splines or Gaussian processes** in geostatistics, imaging and probabilities,

we will hopefully help the reader to get a deeper understanding of a theory that is central to modern data sciences.

[Feydy, [Geometric data analysis, beyond convolutions](#)]

Introducing Theory Space

Direction Space



x = Direction

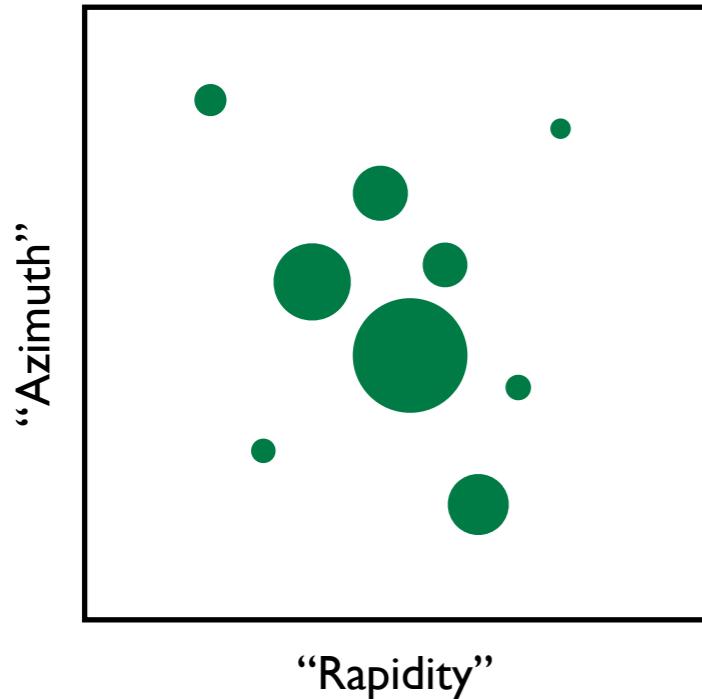
= Angular Distance

$$n_i^\mu = \frac{p_i^\mu}{E_i} = (1, \hat{n})^\mu$$

$$\theta_{ij} = \sqrt{2n_i^\mu n_{j\mu}}$$

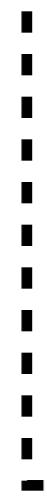
(for massless particles)

Direction Space Distribution



● = Weighted Direction

— = Angular Distance



★ = Event

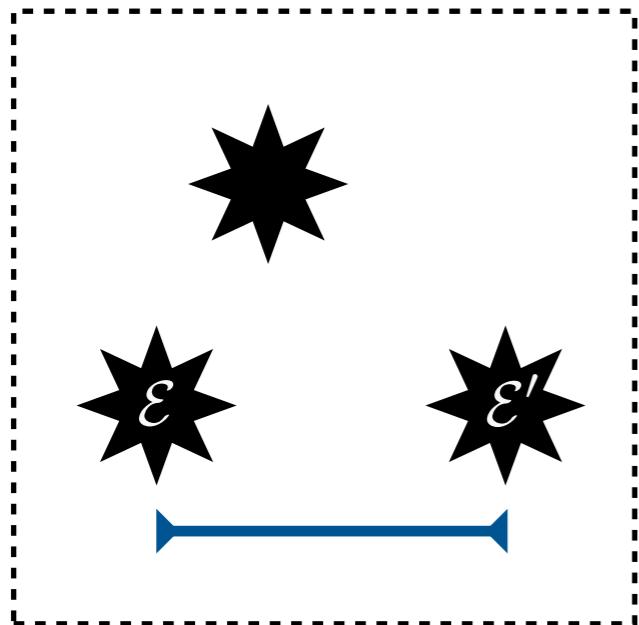
$$n_i^\mu = \frac{p_i^\mu}{E_i} = (1, \hat{n})^\mu$$

$$w_i = E_i$$

$$\theta_{ij} = \sqrt{2n_i^\mu n_{j\mu}}$$

(for massless particles)

Event Space



★ = Event
↔ = EMD
Energy Mover's Distance

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

$$\text{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f\}} \sum_i \sum_j f_{ij} \theta_{ij}$$

(for equal total energy)

[Komiske, Metodiev, JDT, PRL 2019]

Event Space Distribution



= Weighted Event

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

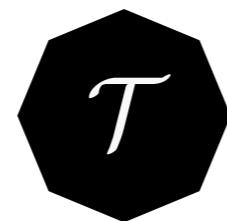
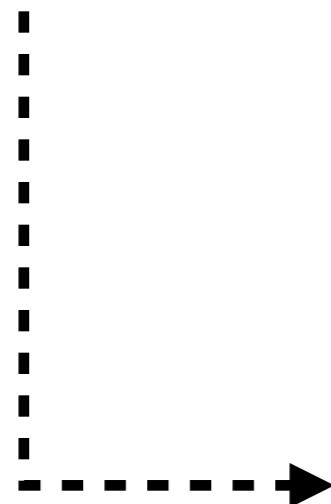
$$w_a = \sigma_a$$

= EMD

Energy
Mover's Distance

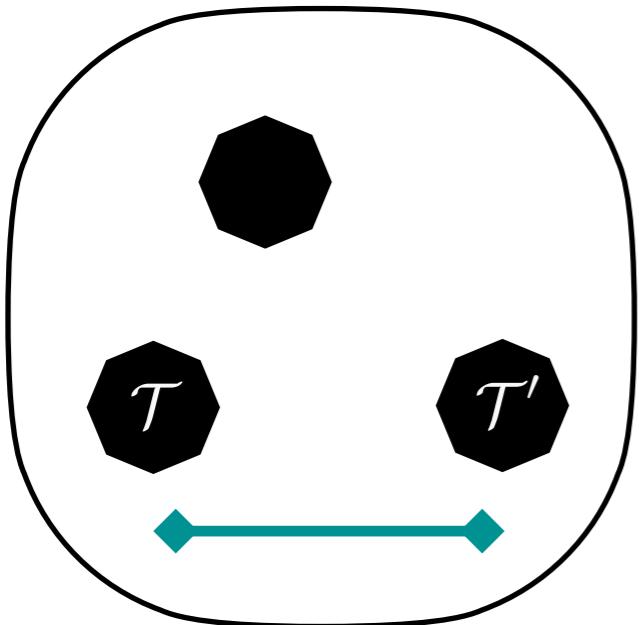
$$\text{EMD}(\mathcal{E}, \mathcal{E}') = \min_{\{f\}} \sum_i \sum_j f_{ij} \theta_{ij}$$

(for equal total energy)



= Theory

Theory Space



● = Theory

↔ = ΣMD
Cross-Section
Mover's Distance

$$\mathcal{T}(\mathcal{E}) = \sum_a \sigma_a \delta(\mathcal{E} - \mathcal{E}_a)$$

$$\Sigma\text{MD}(\mathcal{T}, \mathcal{T}') = \min_{\{\mathcal{F}\}} \sum_a \sum_b \mathcal{F}_{ab} \text{EMD}(\mathcal{E}_a, \mathcal{E}'_b)$$

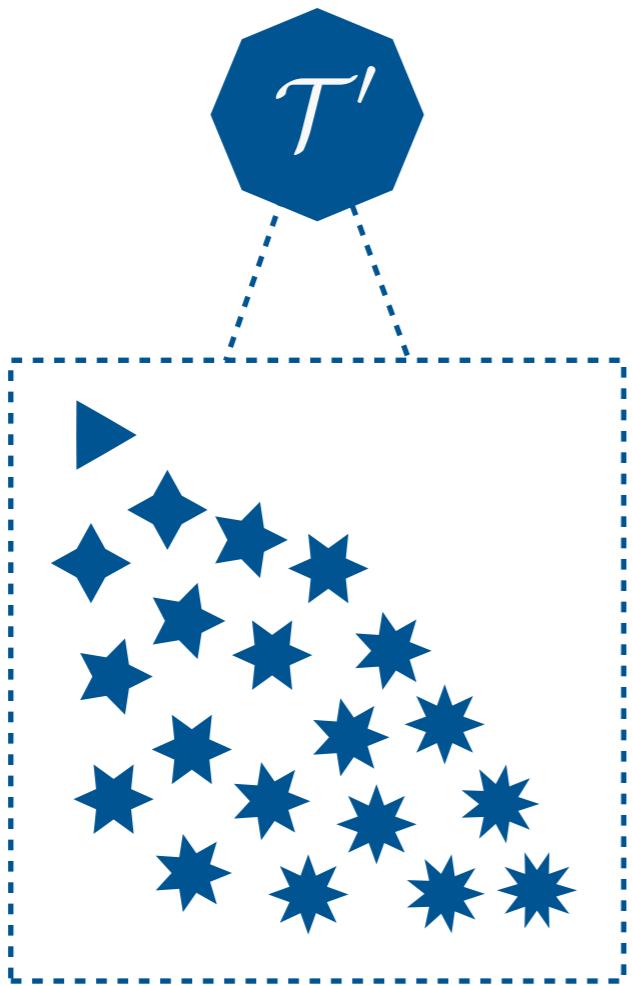
(for equal total xsec)

A distance between theories!

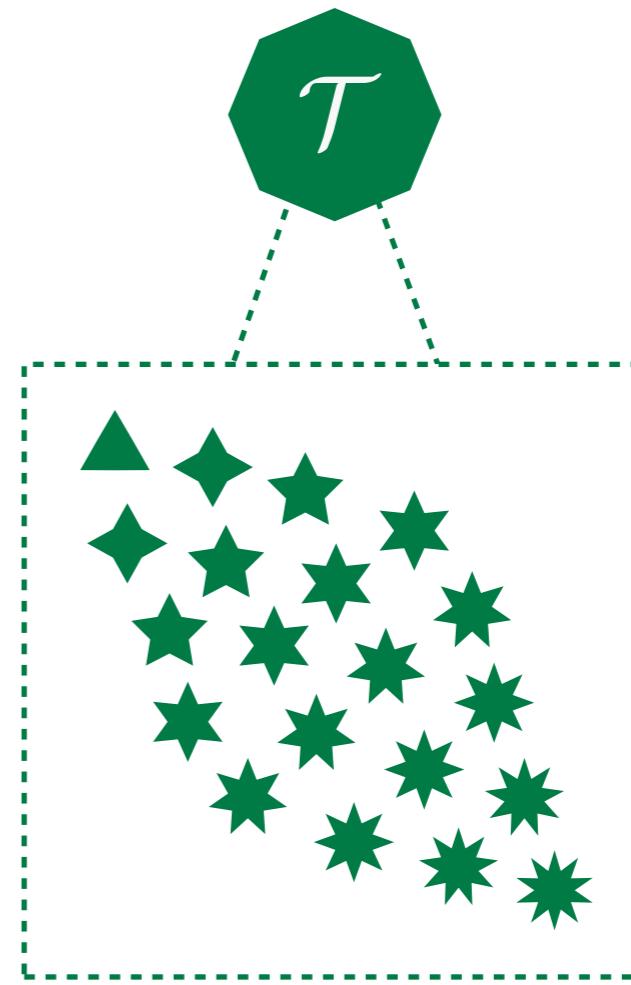
(e.g. EMD : N-jettiness :: ΣMD : k-eventiness)

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

Theory Prime: In-Medium QCD



Theory: Vacuum QCD



ΣMD
 \iff

*Optimal transportation plan defines mapping
between in-medium jets and vacuum jets!*