

# Quantum (Inspired) Algorithms for Collider Physics

Jesse Thaler



QuantHEP Seminar — November 3, 2021

# 2021 SNOWMASS WORKSHOP ON QUANTUM COMPUTING FOR HIGH-ENERGY PHYSICS

DECEMBER 1-3, 2021  
Virtual Event

## QUANTUM MACHINE LEARNING - DATA ANALYSIS - SIMULATION

This workshop aims to bring HEP scientists currently working on or interested in quantum computing applications to HEP and showcase state-of-the-art algorithms for data analysis, and simulation applications.

**Call for abstracts open until November 17th at the Indico website.**  
<https://indico.phy.ornl.gov/event/144/>

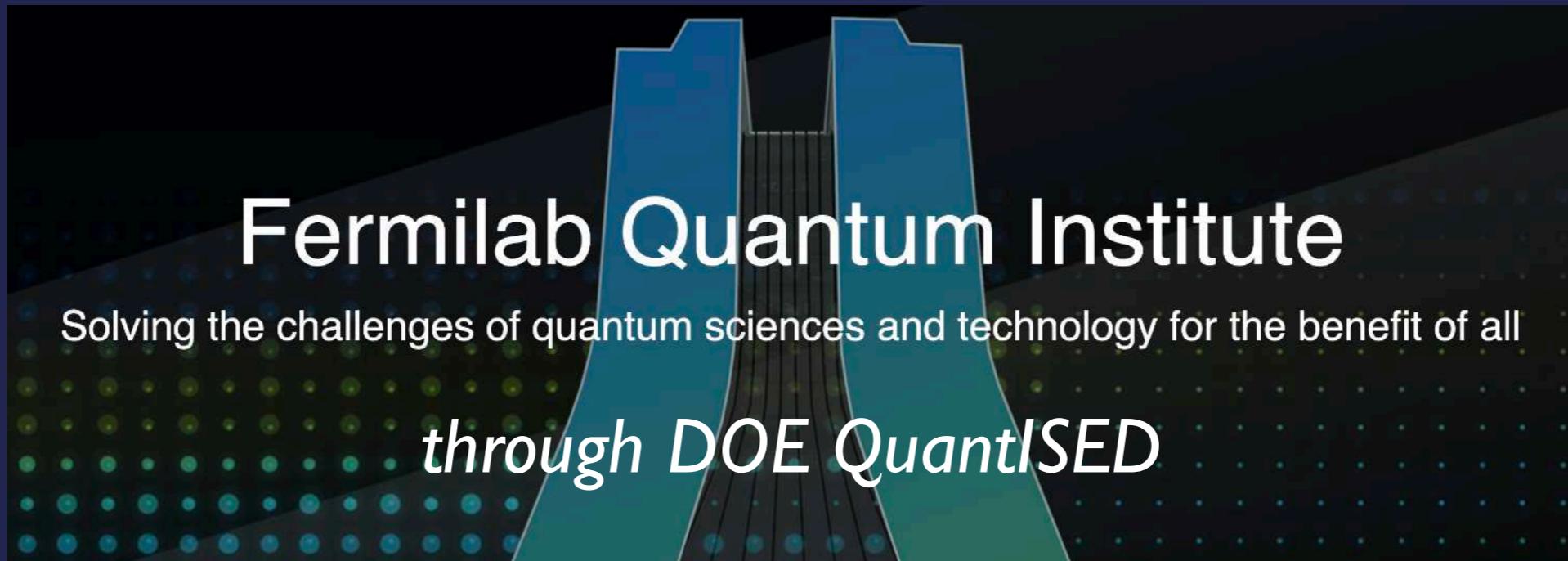
**Questions? Contact the Workshop Chairs:**  
Andrea Delgado (delgadoa@ornl.gov)  
Jean-Roch Vlimant (jvlimant@caltech.edu)

**Local Organizing Committee**

Marcel Demarteau	Kathleen Hamilton
Raphael Pooser	Alex McCaskey



C<sup>2</sup>QA  
Co-design Center for  
Quantum Advantage



A dark blue banner with a textured background of green and blue dots. In the center, the text "Fermilab Quantum Institute" is written in a large, white, serif font. Below it, the tagline "Solving the challenges of quantum sciences and technology for the benefit of all" is in a smaller, white, sans-serif font. At the bottom, the text "through DOE QuantISED" is written in a white, italicized, sans-serif font.

# 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]

# Why “Inspired”?

For the foreseeable future, data collected from colliders like the LHC will be **classical**

Depending on the quantum computing model, **classical data analysis** may or may not be more efficient with **quantum algorithms**

But **quantum principles** (e.g. superposition) and **quantum challenges** (e.g. data loading) have already inspired **new classical algorithms**

*First, evangelizing for QIS/HEP...*

*Slides from 2019 HEPAP presentation*

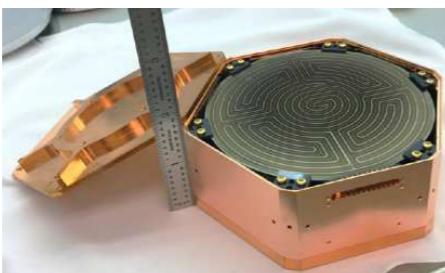
# HEP and the National Quantum Initiative



Quantum: Manipulating individual quantum states  
Using superposition, entanglement, squeezing, etc.

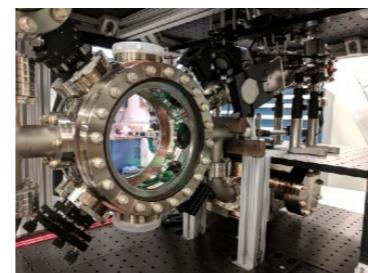
## *Already developing/exploiting Quantum Sensing technologies*

Transition Edge Sensors



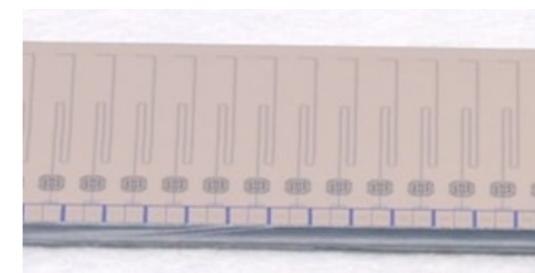
[[SuperCDMS](#)]

Atom Interferometry



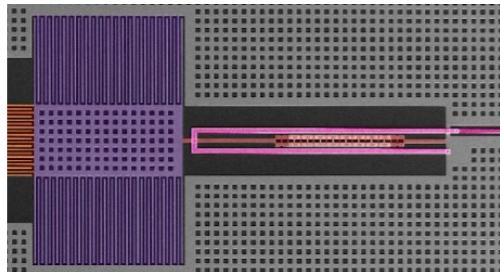
[[MAGIS-100](#)]

Microwave SQUID Multiplexers



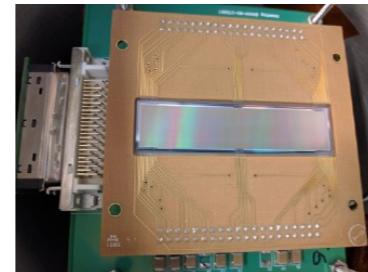
[[Simons Observatory](#)]

Squeezed State Receivers



[[HAYSTAC](#)]

Skipper CCDs



[[SENSEI](#)]

And More!

NMR, superfluid helium,  
graphene, atomic clocks,  
cold atoms, ...

[see [Nov 2018 HEPAP Meeting](#);  
[Quantum Sensing for HEP \(2018\)](#); [2019 Kavli ACP Workshop, Intersections QIS/HEP](#)]

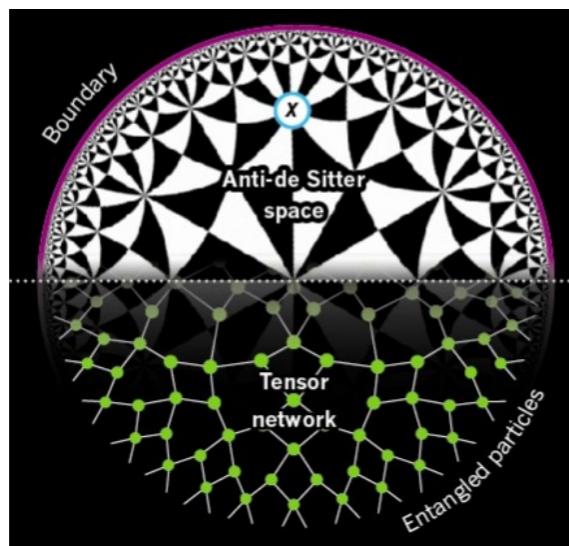
# HEP and the National Quantum Initiative



Quantum: Manipulating individual quantum states  
Using superposition, entanglement, squeezing, etc.

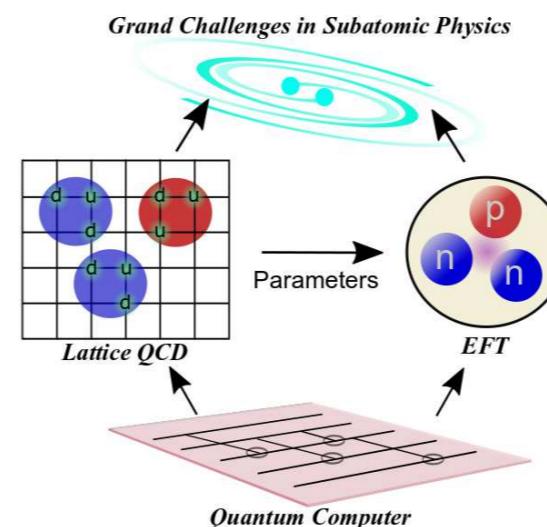
*Fertile intersection between HEP and QIS  
Potentially transformative, requires robust theory/R&D effort*

## Entanglement $\Leftrightarrow$ Geometry



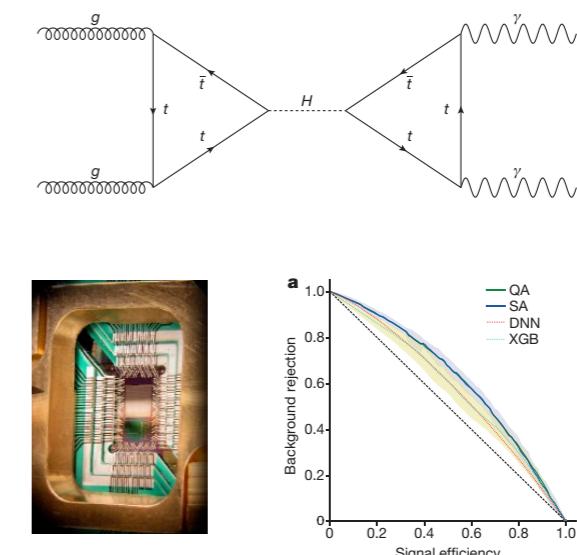
[figure from [Nature 2015](#)]

## Simulation



[figure from [1810.03959](#)]

## Computation/Analysis



[MJVLS, [Nature 2017](#)]

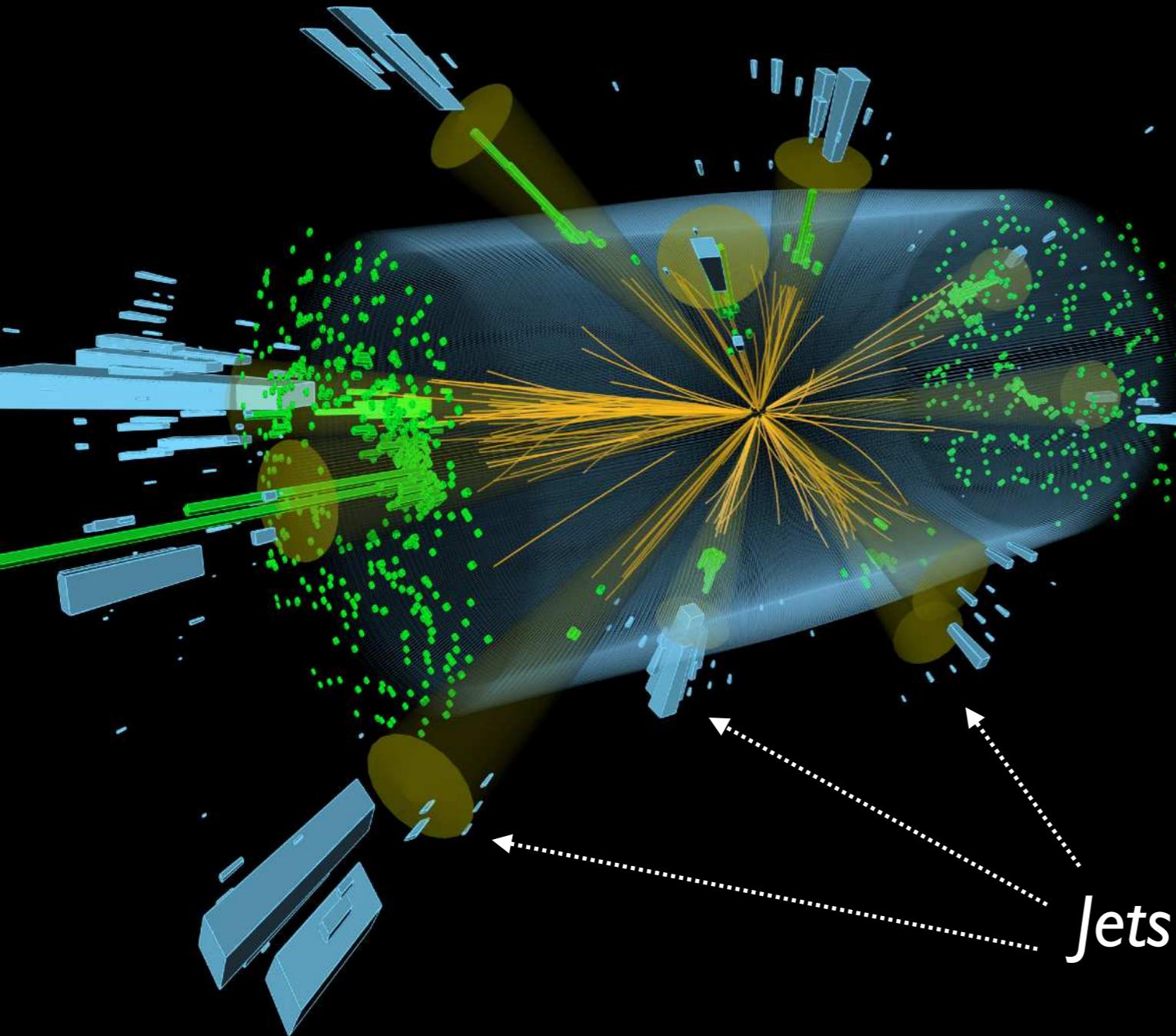
More evangelizing in backup

*Lots of reasons for QIS/HEP excitement!*

*But collider physics data is essentially classical...*

# Collider Event

Every 25 nanoseconds at the LHC



T E H M



$\gamma$

photon



$e^+$

electron



$\mu^+$

muon



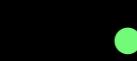
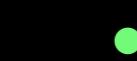
$\pi^+$

pion



$K^+$

kaon



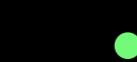
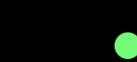
$K_L^0$

K-long



$p/\bar{p}$

proton



$n/\bar{n}$

neutron

elementary

composite

# Collider Event

Every 25 nanoseconds at the LHC

T E H M

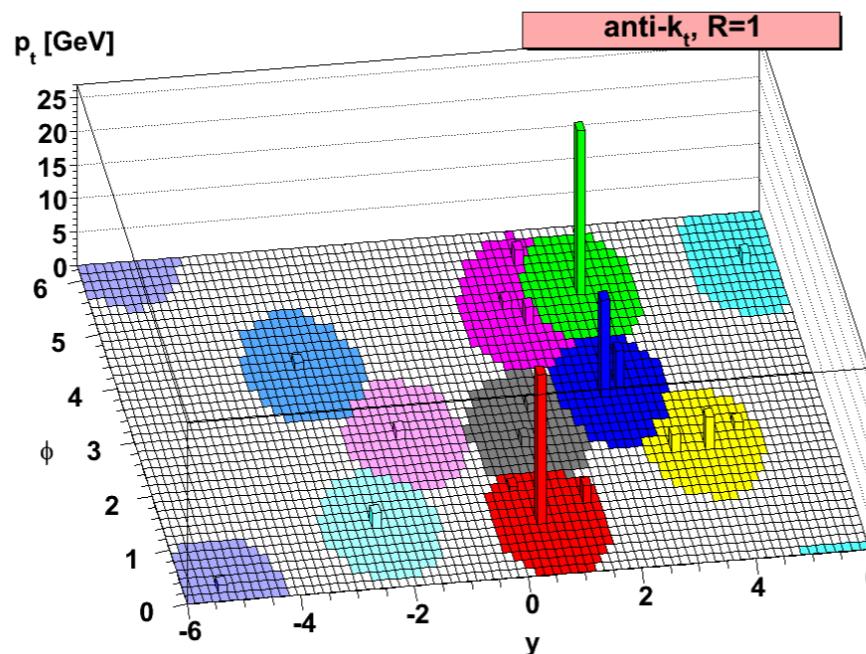


$\gamma$  photon



With  $N$  particles per event, both **quantum & classical** computational cost should (?) scale at least as  $O(N)$

e.g. Sequential Recombination Jet Algorithms:



Naive  $O(N^3)$



Optimized Classical:  
 $O(N^{3/2})$  or  $O(N \log N)$

We work *really hard* to avoid exponentially hard data analysis problems!

[Cacciari, Salam, [PLB 2006](#); Cacciari, Salam, Soyez, [JHEP 2008](#)]

# Collider Event

Every 25 nanoseconds at the LHC

T E H M

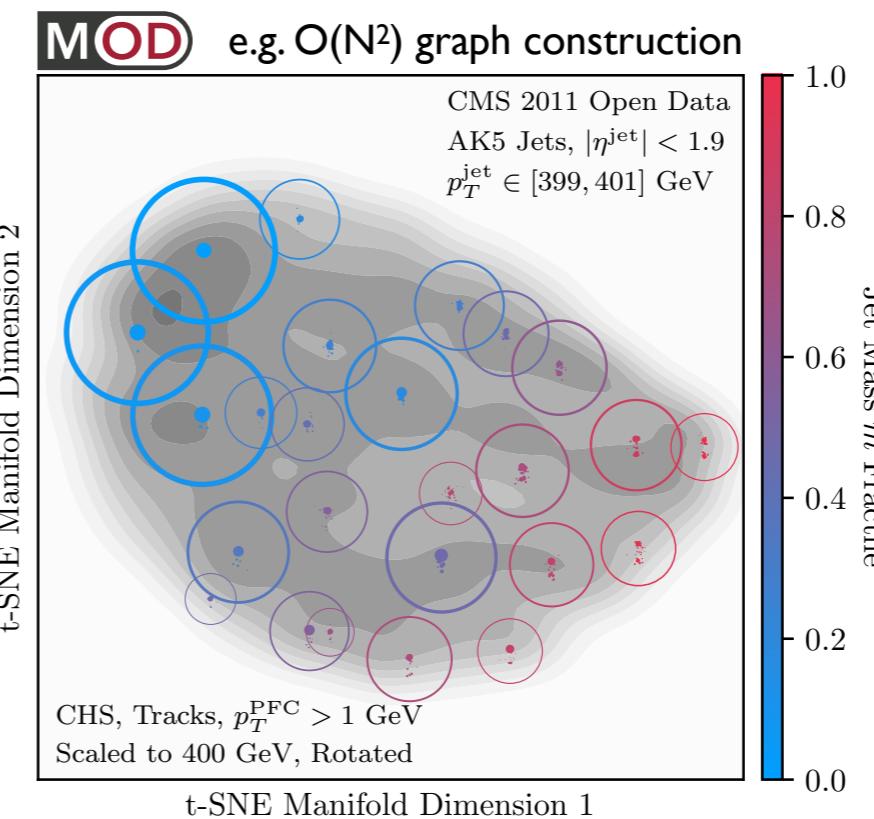
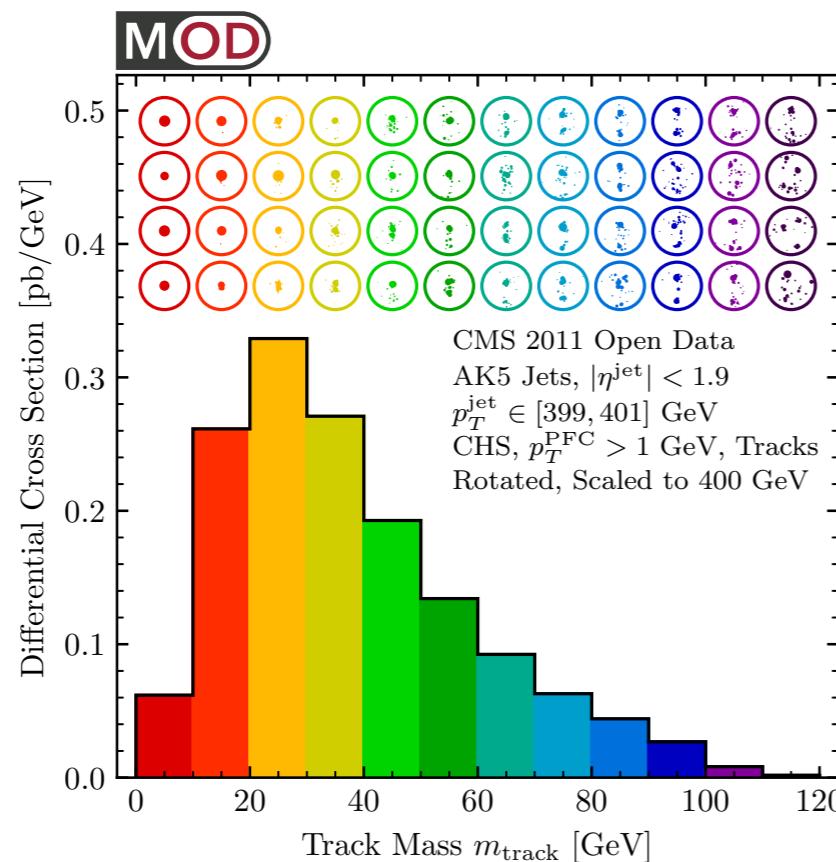


$\gamma$

photon



With  $N$  events per ensemble, cheapest (?) thing we can do is **classically build histograms** at  $O(N)$

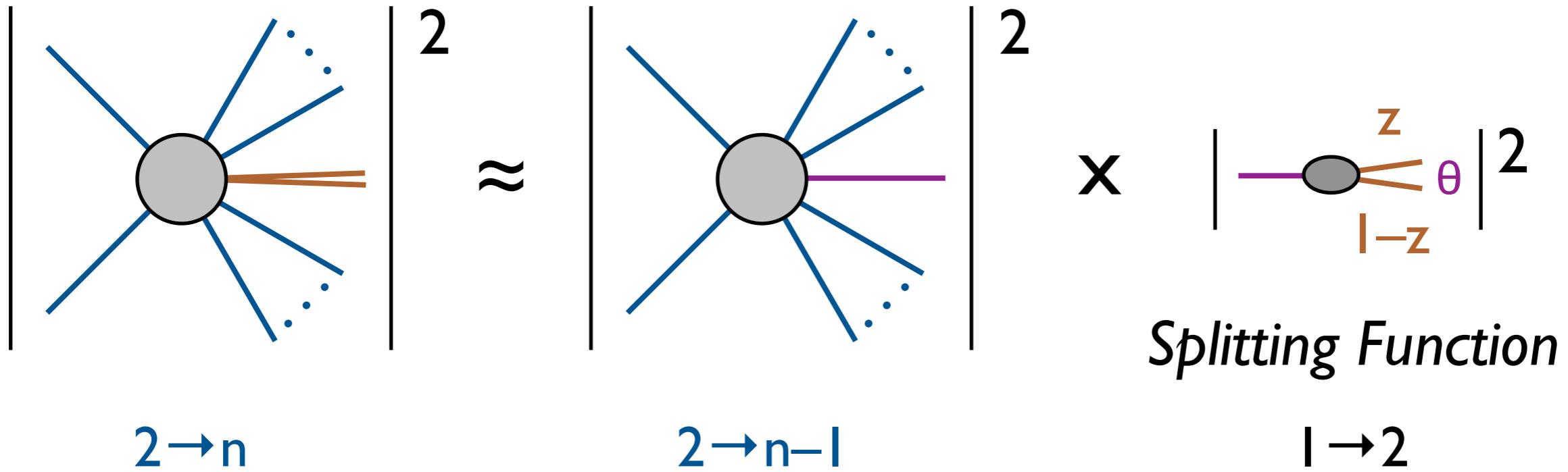


For **quantum advantage**, must start from **harder classical problems**

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

# Factorization Suppresses Quantum Interference

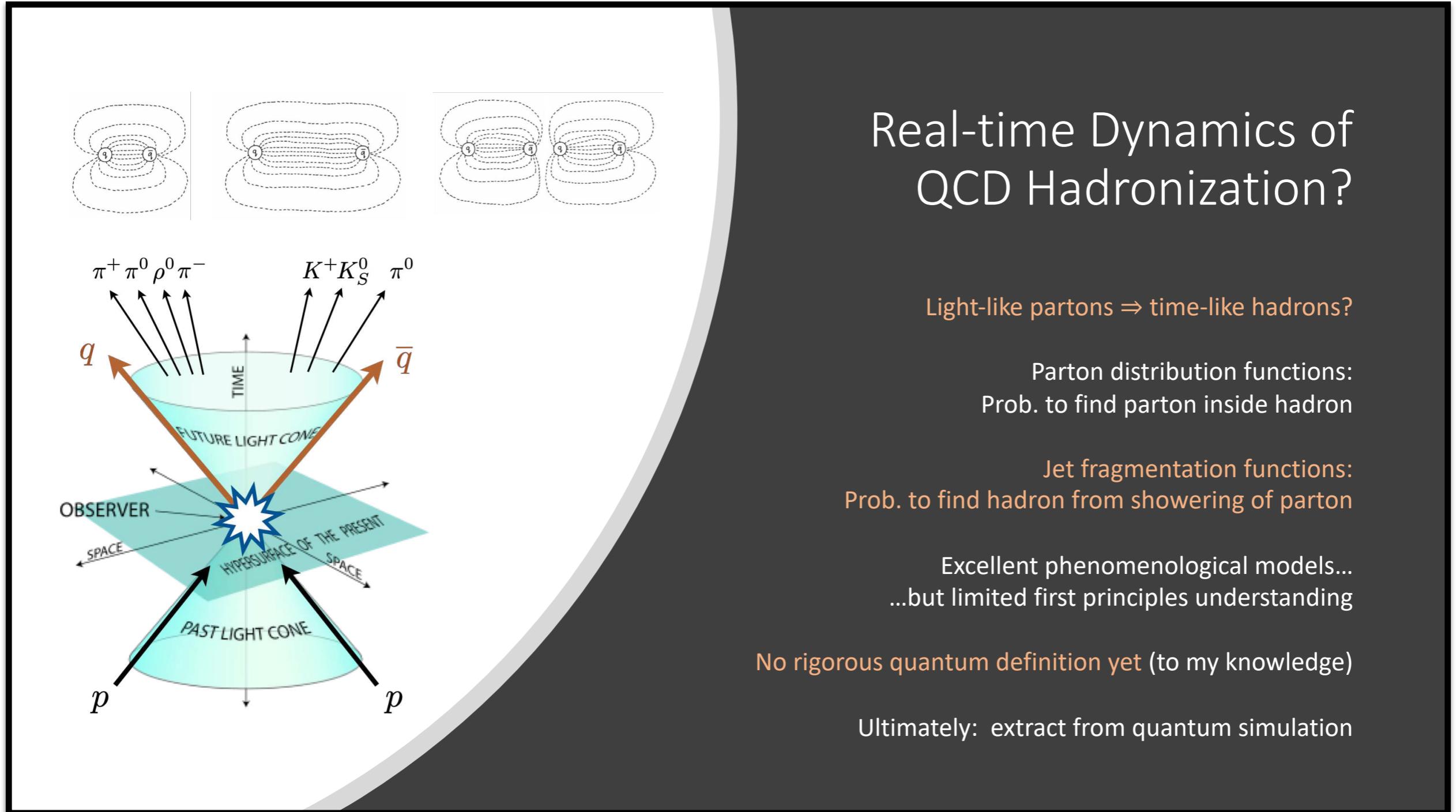
In soft/collinear limit of QCD, aspects of perturbative quantum field theory becomes semi-classical



Roughly same principle allows faster (classical) computation of scattering amplitudes through generalized unitary

[see, however, parton shower progress in Bauer, de Jong, Nachman, Provasoli, [PRL 2021](#); Bepari, Malik, Spannowsky, Williams, [PRD 2021](#), [arXiv 2021](#)]

# Dreaming: Non-Perturbative Jet Fragmentation



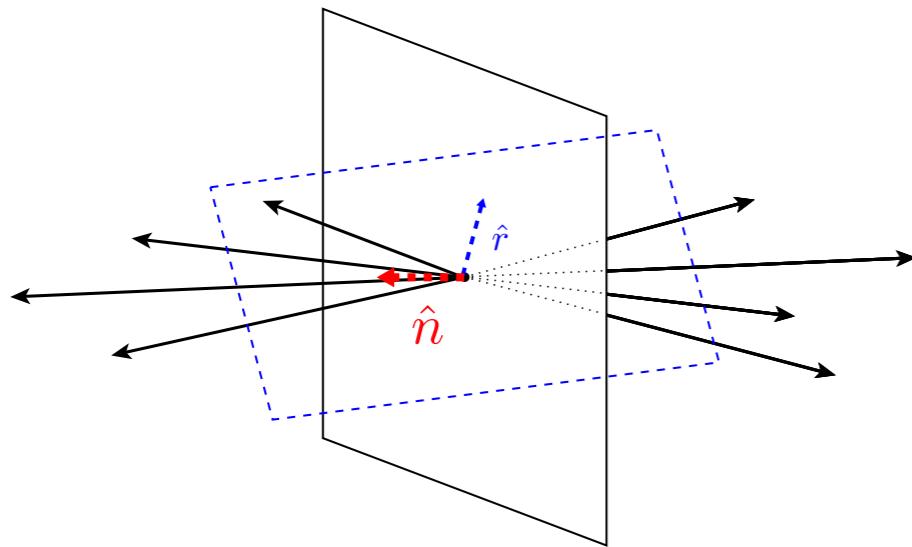
[slide from C<sup>2</sup>QA meet & greet]

*Until then, leveraging quantum inspirations!*

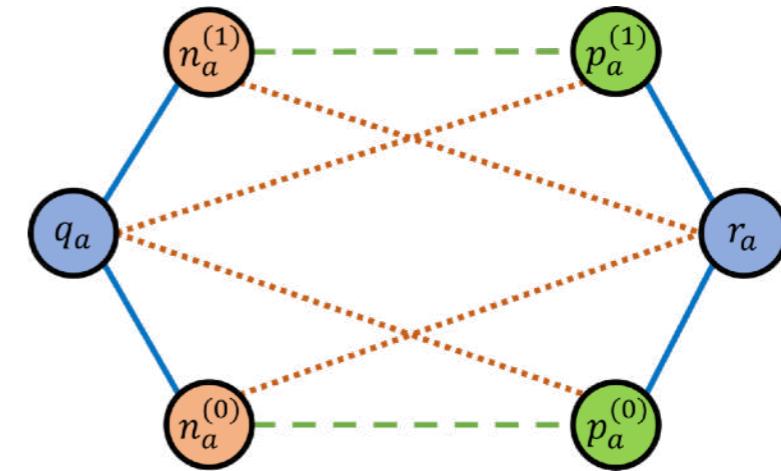
*Even though practical algorithms are currently classical...*

# Four Quantum (Inspired) Anecdotes

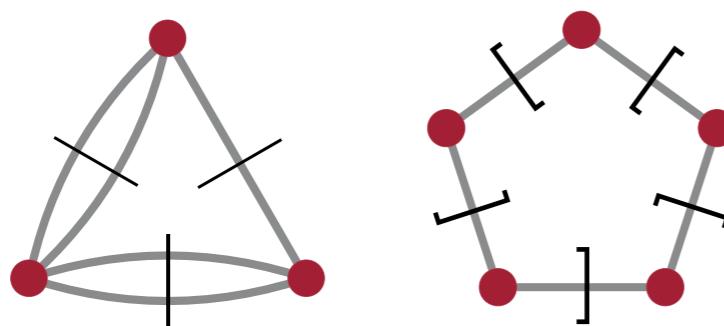
## Challenge of Data Loading



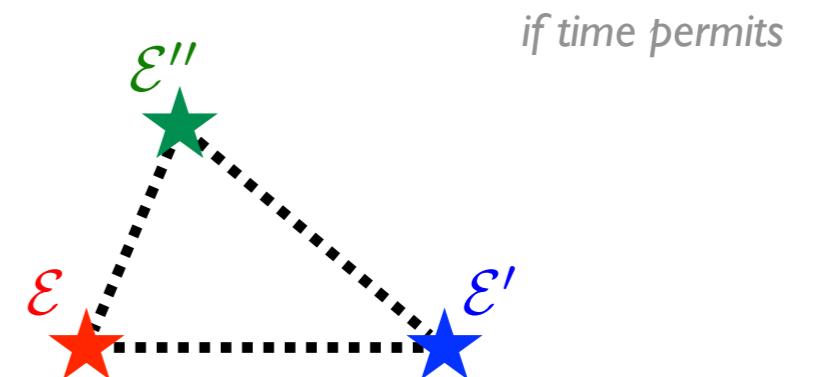
## Degeneracy Engineering



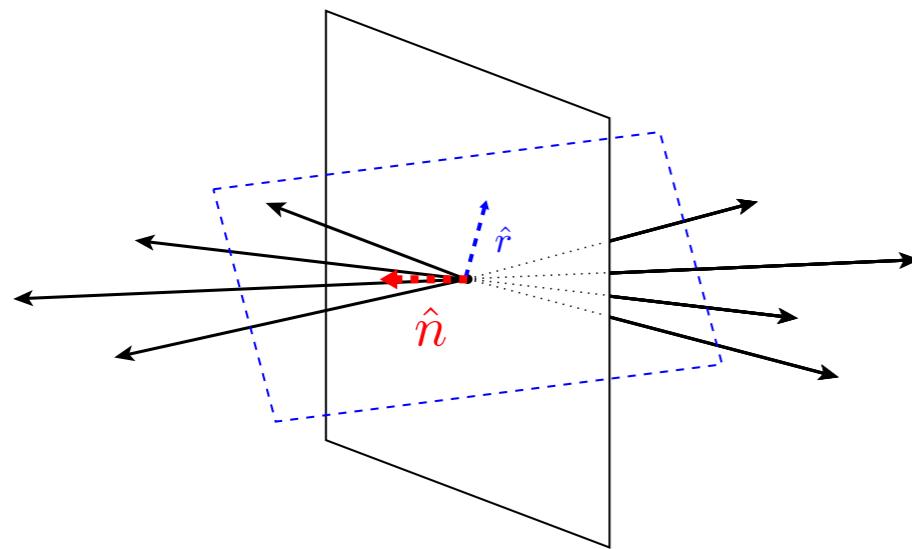
## Superposition for Graphs



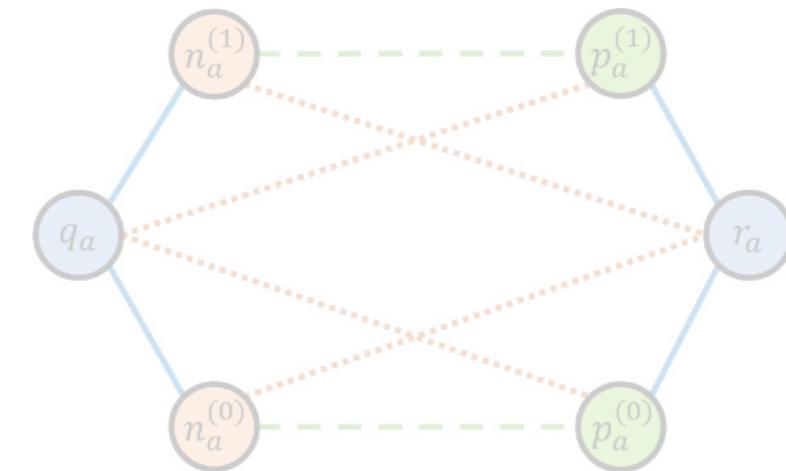
## Optimal Transport



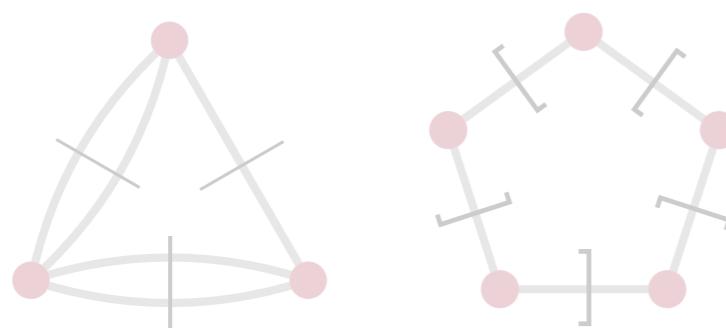
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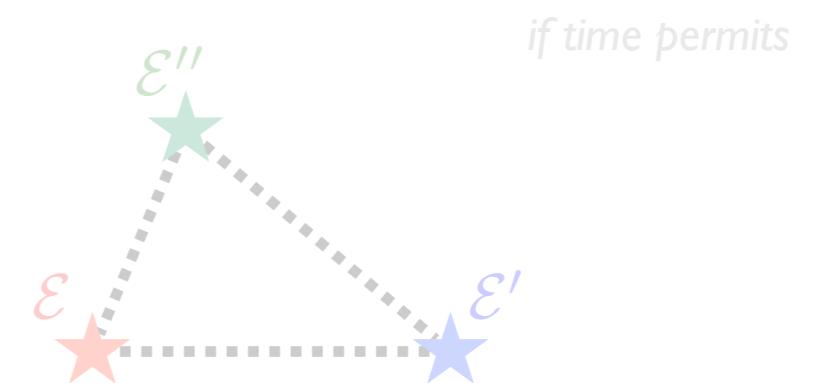
## Degeneracy Engineering



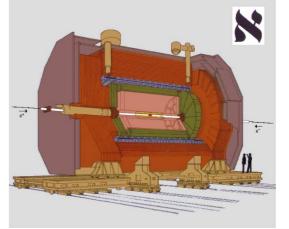
## Superposition for Graphs



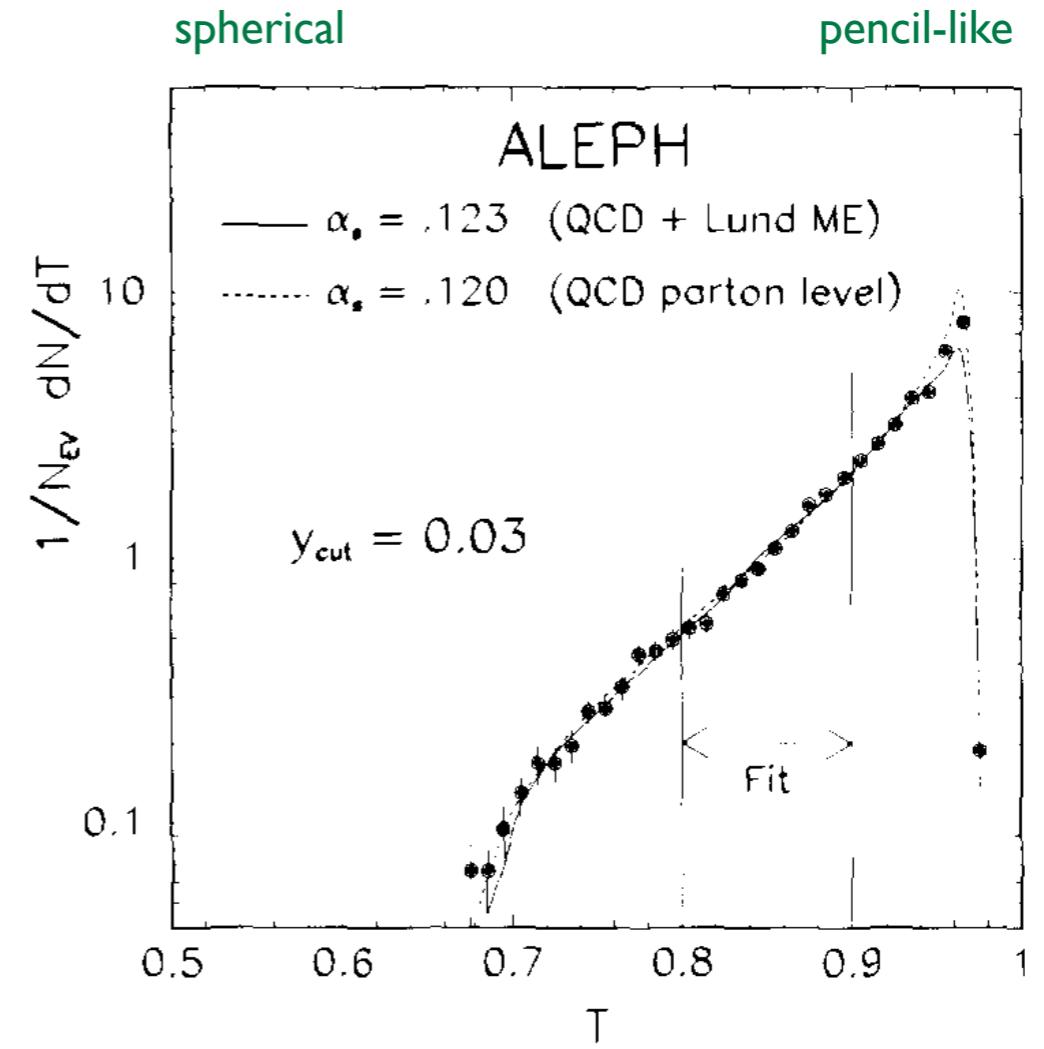
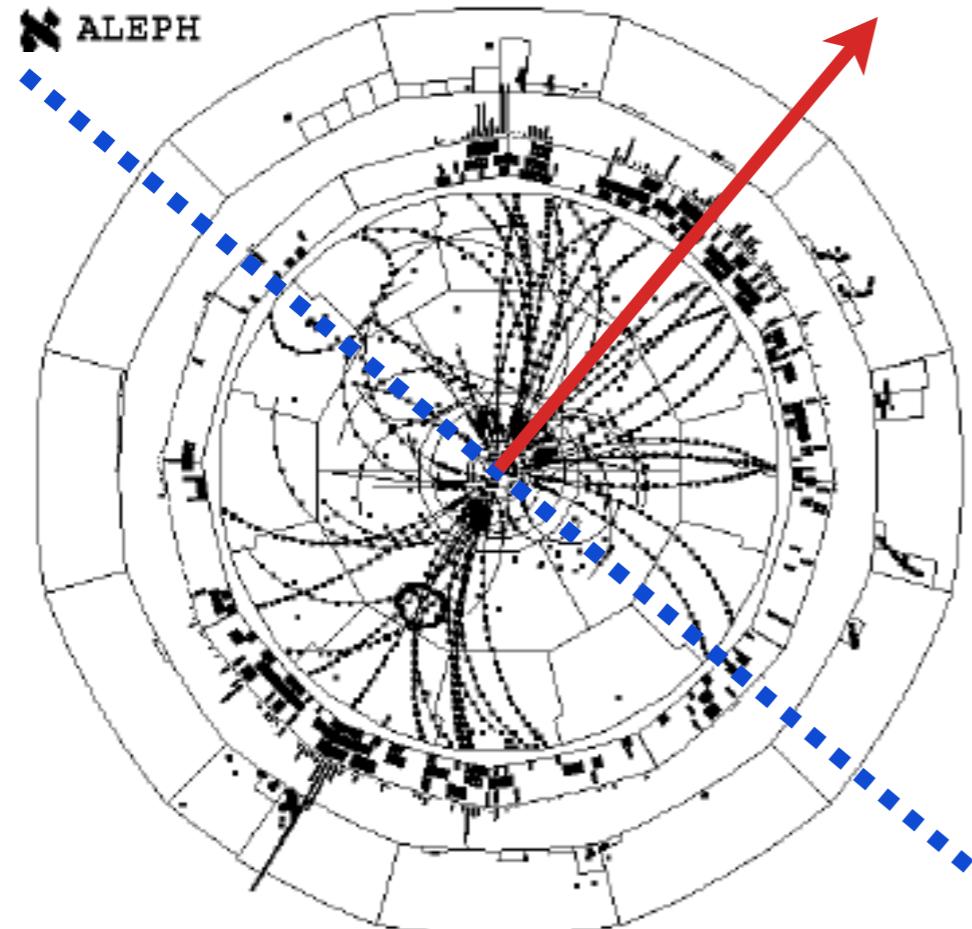
## Optimal Transport



# Jet Clustering with Thrust

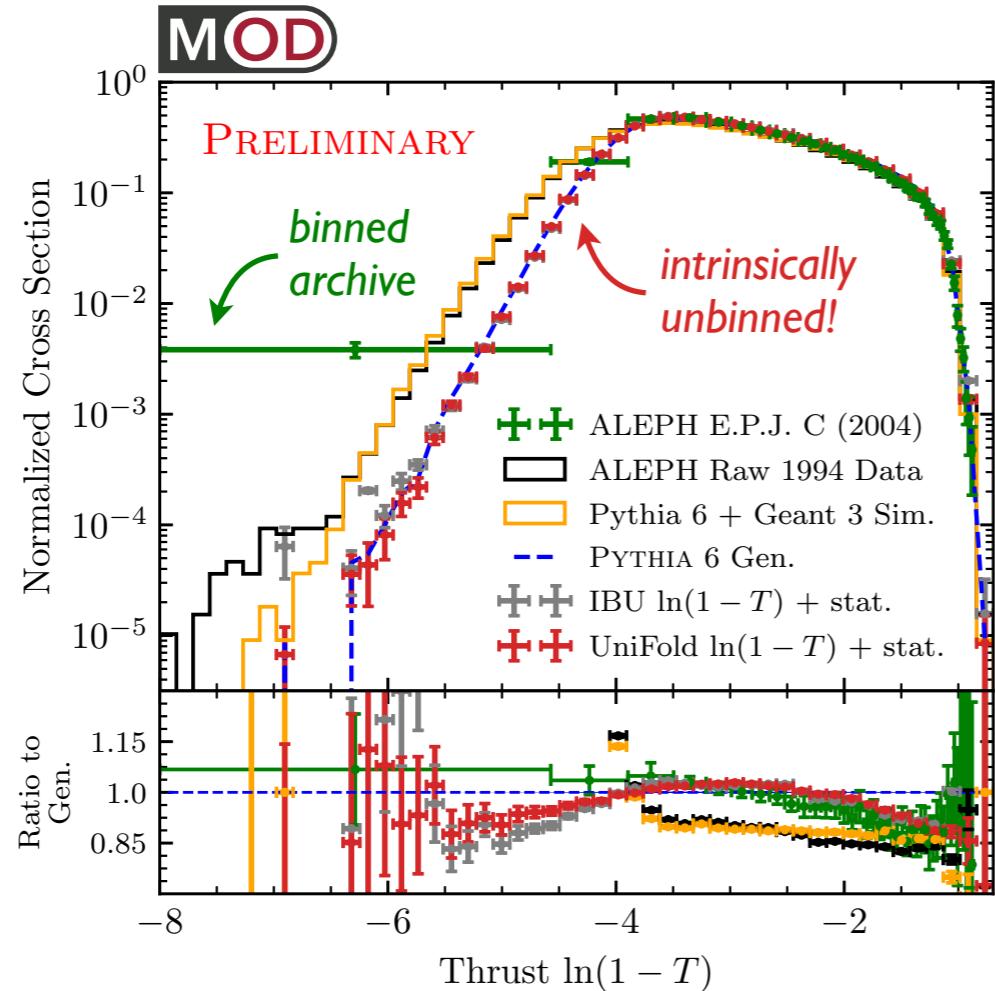
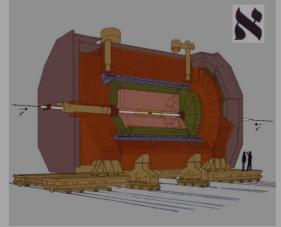


Classic hemisphere partitioning for  $e^+e^-$  colliders



[Brandt, Peyrou, Sosnowski, Wroblewski, [PL 1964](#); Farhi, [PRL 1977](#); ALEPH, [PLB 1991](#)]

# Jet Clustering with Thrust

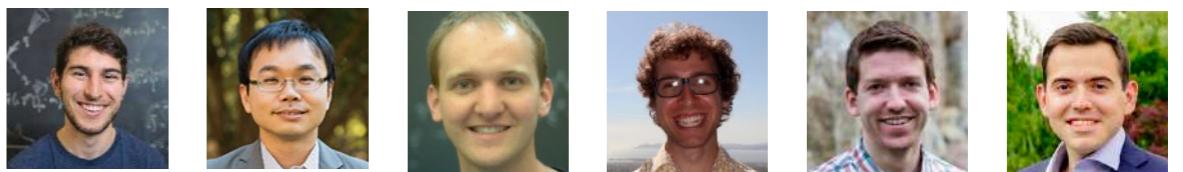


Back to the Future with  
ALEPH Archival Data



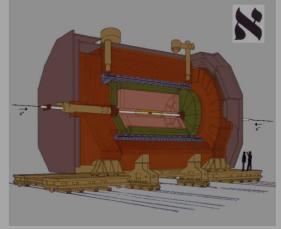
*Multi-dimensional unbinned  
detector corrections  
via machine learning*

[talk by Badea, [ICHEP 2020](#); cf. ALEPH, [EPJC 2004](#)]  
[using Andreassen, Komiske, Metodiev, Nachman, JDT, [PRL 2020](#)]  
[see Badea, Baty, Chang, Innocenti, Maggi, McGinn, Peters, Sheng, JDT, Lee, [PRL 2019](#)]  
[for unbinned archival strategy see Arratia, et al., [arXiv 2021](#)]



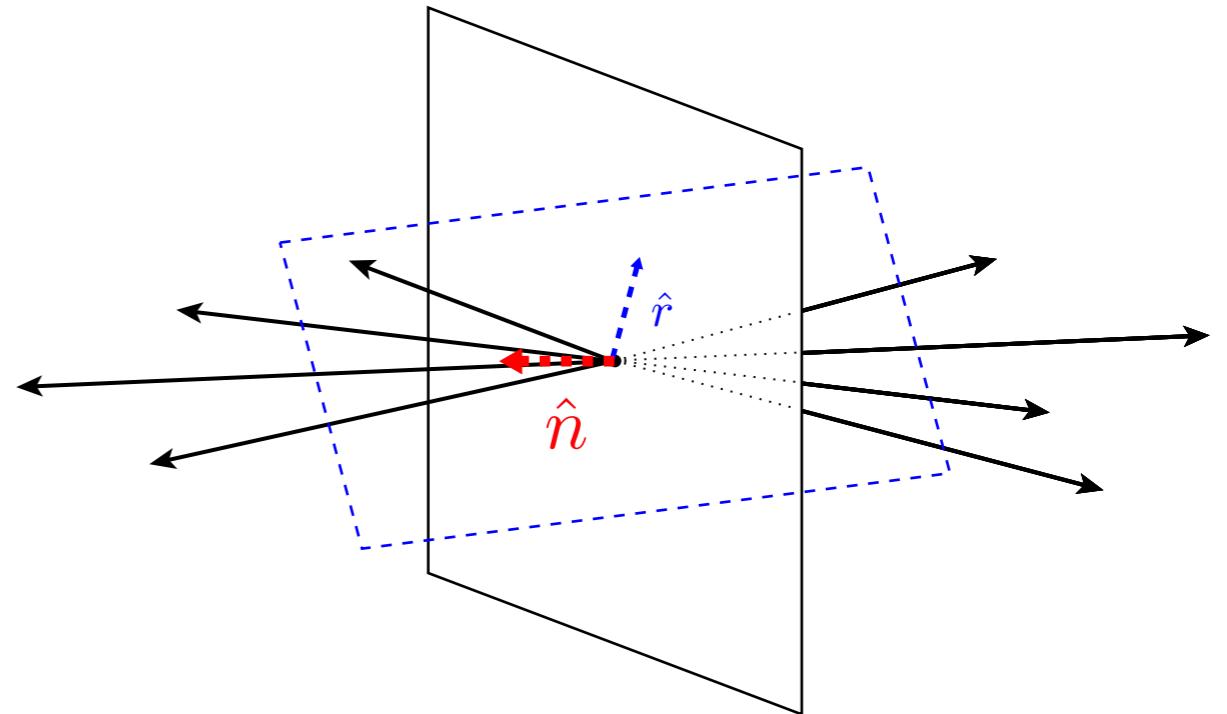
[Brandt, Peyrou, Sosnowski, Wroblewski, [PL 1964](#); Farhi, [PRL 1977](#); ALEPH, [PLB 1991](#)]

# Jet Clustering with Thrust



Best Known Classical Thrust Algorithm:  $O(N^3)$  for  $N$  particles

$$T = \max_{|\hat{n}|=1} \frac{\sum_{i=1}^N |\hat{n} \cdot \vec{p}_i|}{\sum_{i=1}^N |\vec{p}_i|}$$



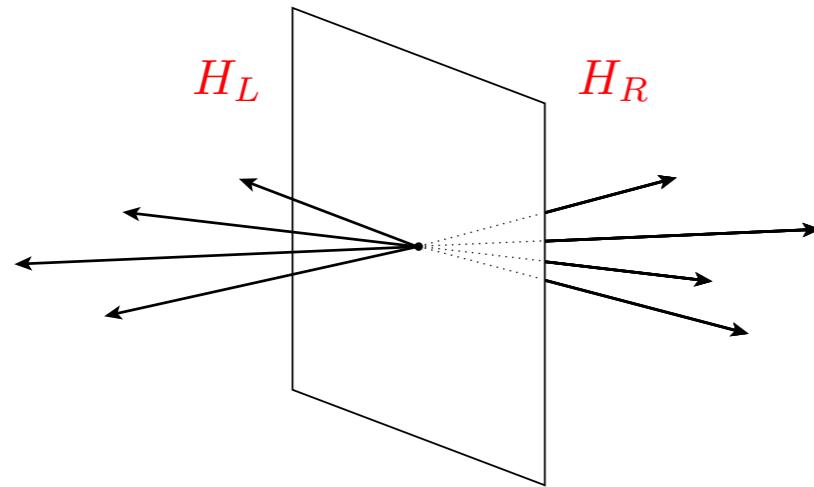
Trick: Recast **axis finding** as **partition finding**

$$O(N^3) = O(N^2)_{\text{partitions}} \times O(N)_{\text{evaluation}}$$

[Yamamoto, JCP 1983; default algorithm in Pythia 8]

[Brandt, Peyrou, Sosnowski, Wroblewski, PL 1964; Farhi, PRL 1977; ALEPH, PLB 1991]

# Quantum Jet Clustering



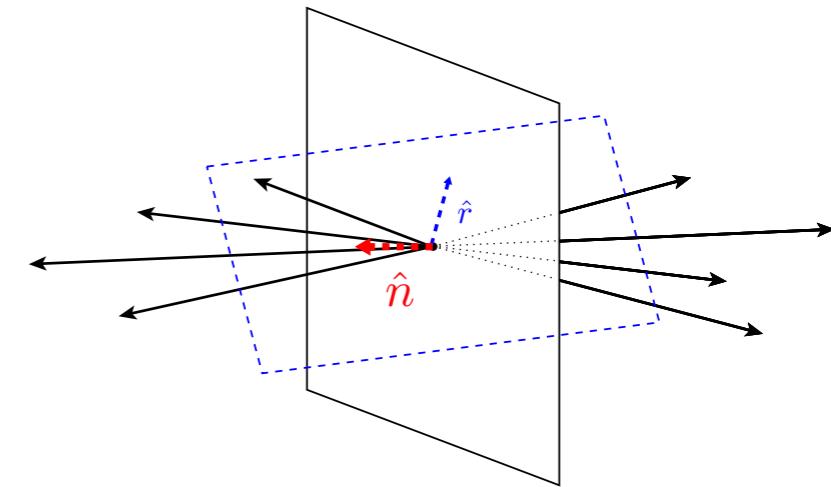
Naive Partitioning:  $O(2^N)$



QUBO for Quantum Annealing

Key lesson:  
Very good *classical heuristics*

Dual Formulations



Best Known Classical:  $O(N^3)$



$O(N^2)$  with Grover-style Search

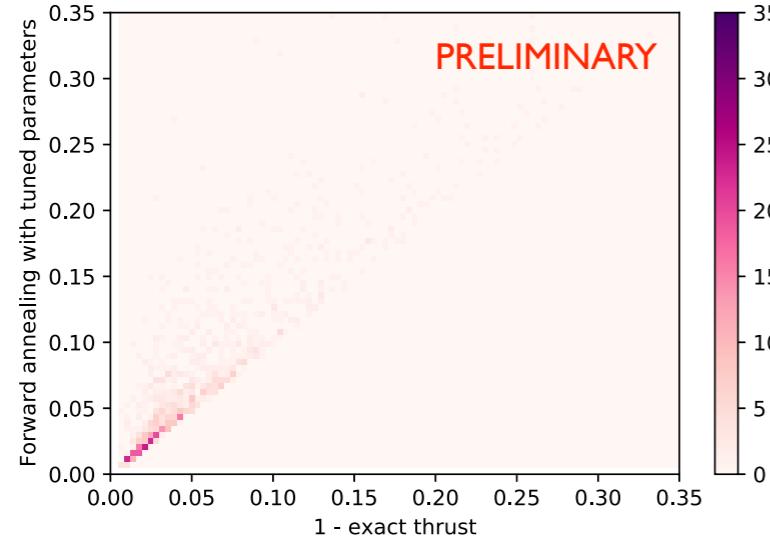
Key lesson: *Quantum algorithm limited by  $O(N)$  classical data loading*

[Wei, Naik, Harrow, JDT, [PRD 2020](#)]  
[see also Pires, Omar, Seixas, [arXiv 2020](#); Pires, Bargassa, Seixas, Omar, [arXiv 2021](#)]

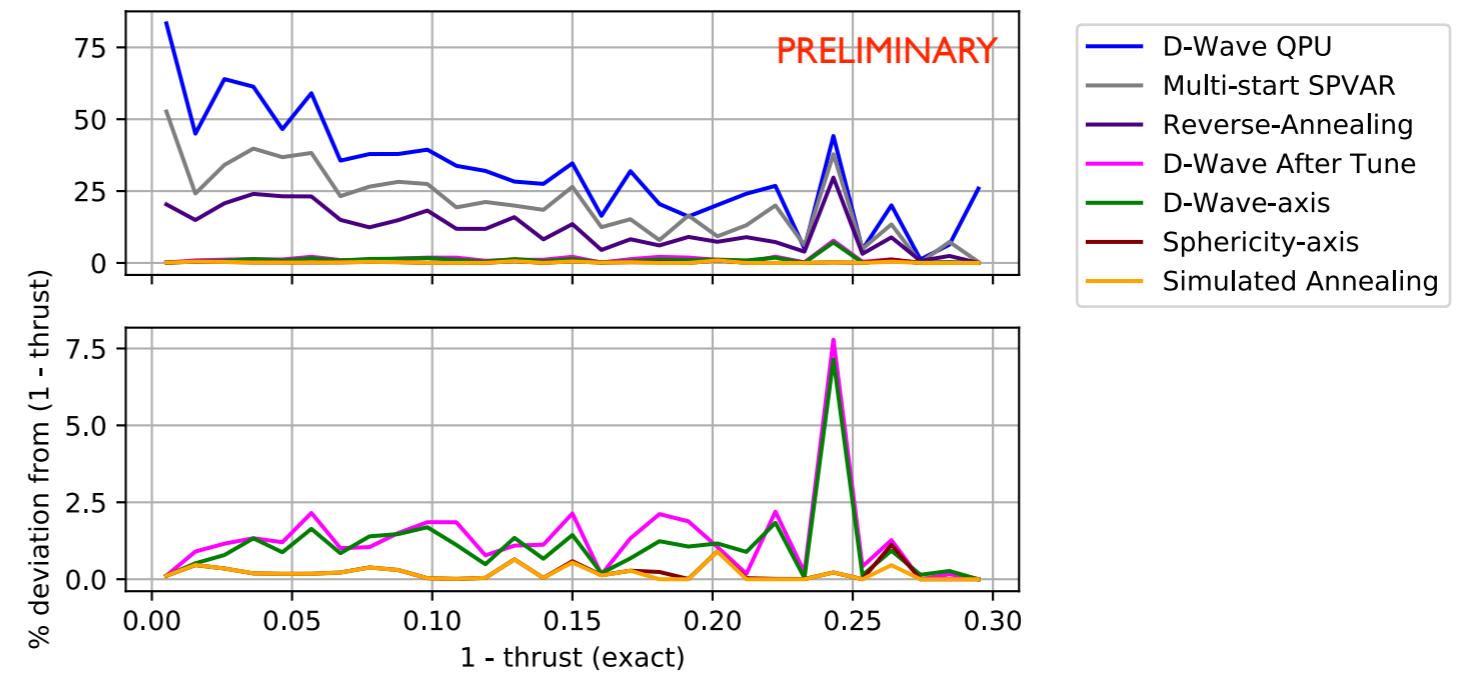


# Quantum Annealing for Thrust

D-Wave Advantage can handle  $O(100)$  particles



Good correlation for  
tuned annealing schedule!



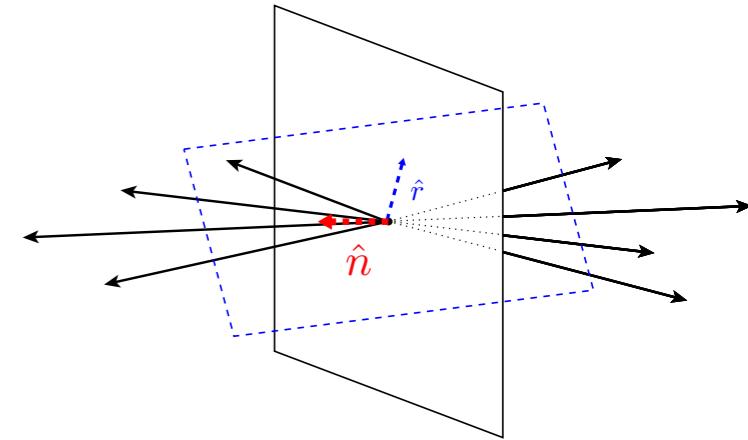
But iterative heuristic  
does comparably well

[Delgado, JDT, in progress]  
[heuristic is default algorithm in Pythia 6]



# Quantum Search for Thrust

Grover search to find optimal partition



1. Randomly pick indices  $m, n$  and set `curr_max` =  $(m, n)$ .

2. Compute  $p\_sum = \frac{1}{2} \sum_{i=1}^{2N} |\vec{p}_i|$ .

3. Set `iter_count` = 0 and `max_it` = 1.

4. While `iter_count` <  $O(N)$ :

(a) While `max_it` <  $O(N)$ :

i. Prepare the initial state  $|\psi_0\rangle = \frac{1}{\sqrt{2N}} \sum_{i,j=1}^{2N} |i\rangle |j\rangle |\vec{0}\rangle |\vec{0}\rangle |\hat{0}\rangle |\vec{0}\rangle |0\rangle$ .

ii. Choose `grov_steps` uniformly at random from  $\{0, 1, \dots, \text{max\_it} - 1\}$ .

iii. Let `iter_count` = `iter_count` + `grov_steps`.

iv. Repeat `grov_steps` times:

A. Call subroutine `COMP_T` to compute  $T_{ij}$ :

$$|i\rangle |j\rangle |\vec{0}\rangle |\vec{0}\rangle |\hat{0}\rangle |\vec{0}\rangle |0\rangle \mapsto |i\rangle |j\rangle |\vec{0}\rangle |\vec{0}\rangle |\hat{0}\rangle |\vec{0}\rangle |T_{ij}\rangle .$$

B. Reflect about states with  $T_{ij} > T_{\text{curr\_max}}$  with a phase factor:

$$|i\rangle |j\rangle |\vec{0}\rangle |\vec{0}\rangle |\hat{0}\rangle |\vec{0}\rangle |T_{ij}\rangle \mapsto (-1)^{\Theta(T_{ij} - T_{\text{curr\_max}})} |i\rangle |j\rangle |\vec{0}\rangle |\vec{0}\rangle |\hat{0}\rangle |\vec{0}\rangle |T_{ij}\rangle .$$

C. Uncompute the  $T_{ij}$  register to obtain state:  $(-1)^{\Theta(T_{ij} - T_{\text{curr\_max}})} |i\rangle |j\rangle |\vec{0}\rangle |\vec{0}\rangle |\hat{0}\rangle |\vec{0}\rangle |0\rangle$ .

D. Reflect about the initial state using  $R_0 = 2|\psi_0\rangle\langle\psi_0| - I^{\otimes 7}$ .

v. Measure the  $\{i, j, T_{ij}\}$  registers to obtain  $\{k, \ell, T_{k\ell}\}$ ; if  $T_{k\ell} > T_{\text{curr\_max}}$ , set `curr_max` =  $(k, \ell)$  and break.

(b) Let `max_it` =  $\mu \times \text{max\_it}$ , where  $\mu$  is a constant between 1 and  $4/3$ .

5. Measure the  $\{i, j, T_{ij}\}$  registers to obtain  $\{k, \ell, T_{k\ell}\}$ ; if  $T_{k\ell} > T_{\text{curr\_max}}$ , set `curr_max` =  $(k, \ell)$ .

I How expensive  
is this?

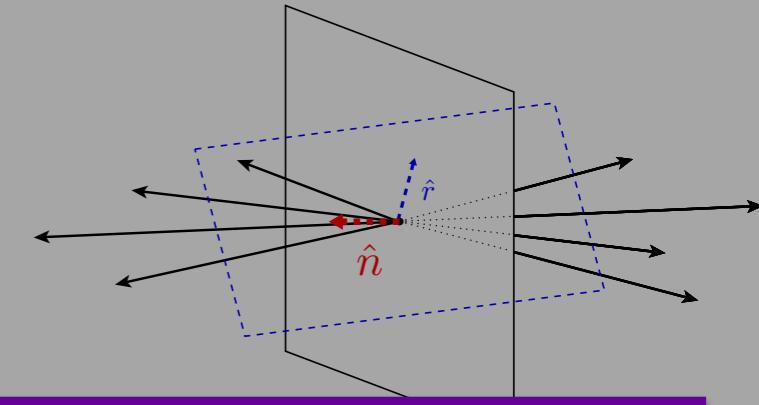
Grover over  
 $N^2$  partitions  
in  $O(N)$

[Wei, Naik, Harrow, JDT, PRD 2020]



# Quantum Search for Thrust

*Grover search to find optimal partition*



**Grover over  
 $N^2$  partitions  
in  $O(N)$**

1. Randomly sample  $i, j$
2. Compute  $\vec{p}_i, \vec{p}_j$
3. Set  $\text{it} = 0$
4. While  $\text{it} < \text{max\_it}$

(a)

1. Load  $\vec{p}_i, \vec{p}_j$  using LOOKUP:

$$|i\rangle |j\rangle |\vec{0}\rangle |\vec{0}\rangle |\hat{0}\rangle |\vec{0}\rangle |0\rangle \mapsto |i\rangle |j\rangle |\vec{p}_i\rangle |\vec{p}_j\rangle |\hat{0}\rangle |\vec{0}\rangle |0\rangle .$$

2. Calculate the reference axis via  $\hat{r}_{ij} = (\vec{p}_i \times \vec{p}_j) / |\vec{p}_i \times \vec{p}_j|$ :

$$|i\rangle |j\rangle |\vec{p}_i\rangle |\vec{p}_j\rangle |\hat{0}\rangle |\vec{0}\rangle |0\rangle \mapsto |i\rangle |j\rangle |\vec{p}_i\rangle |\vec{p}_j\rangle |\hat{r}_{ij}\rangle |\vec{0}\rangle |0\rangle .$$

3. Apply SUM, with  $f(\vec{p}_k; \hat{r}_{ij}) = \{\vec{p}_k/2 \text{ if } \hat{r}_{ij} \cdot \vec{p}_k > 0; \vec{0} \text{ if } \hat{r}_{ij} \cdot \vec{p}_k < 0\}$ , to obtain hemisphere momentum  $\vec{P}_{ij}$ :

$$|i\rangle |j\rangle |\vec{p}_i\rangle |\vec{p}_j\rangle |\hat{r}_{ij}\rangle |\vec{0}\rangle |0\rangle \mapsto |i\rangle |j\rangle |\vec{p}_i\rangle |\vec{p}_j\rangle |\hat{r}_{ij}\rangle |\vec{P}_{ij}\rangle |0\rangle .$$

4. Calculate thrust via  $T_{ij} = 2|\vec{P}_{ij}|/\text{p\_sum}$ :

$$|i\rangle |j\rangle |\vec{p}_i\rangle |\vec{p}_j\rangle |\hat{r}_{ij}\rangle |\vec{P}_{ij}\rangle |0\rangle \mapsto |i\rangle |j\rangle |\vec{p}_i\rangle |\vec{p}_j\rangle |\hat{r}_{ij}\rangle |\vec{P}_{ij}\rangle |T_{ij}\rangle .$$

5. Uncompute registers to obtain state:  $|i\rangle |j\rangle |\vec{0}\rangle |\vec{0}\rangle |\hat{0}\rangle |\vec{0}\rangle |T_{ij}\rangle$ .

**Subroutine COMP\_T:**

**I And this?**

- C. Uncompute the  $T_{ij}$  register to obtain state:  $(-1)^{\Theta(T_{ij} - T_{\text{curr\_max}})} |i\rangle |j\rangle |\vec{0}\rangle |\vec{0}\rangle |\hat{0}\rangle |\vec{0}\rangle |0\rangle$ .
- D. Reflect about the initial state using  $R_0 = 2|\psi_0\rangle\langle\psi_0| - I^{\otimes 7}$ .
- v. Measure the  $\{i, j, T_{ij}\}$  registers to obtain  $\{k, \ell, T_{k\ell}\}$ ; if  $T_{k\ell} > T_{\text{curr\_max}}$ , set  $\text{curr\_max} = (k, \ell)$  and break.

(b) Let  $\text{max\_it} = \mu \times \text{max\_it}$ , where  $\mu$  is a constant between 1 and  $4/3$ .

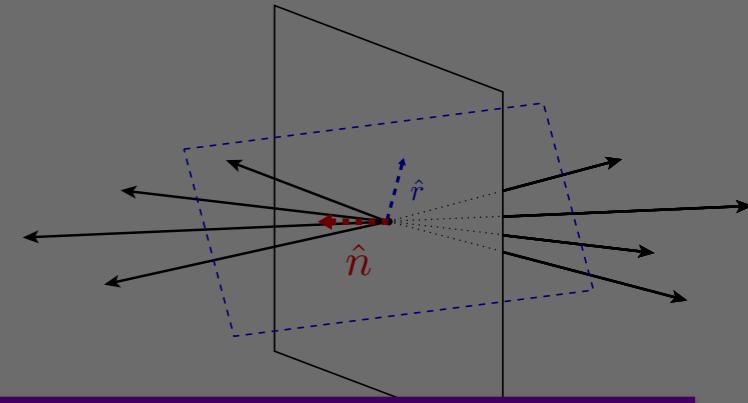
5. Measure the  $\{i, j, T_{ij}\}$  registers to obtain  $\{k, \ell, T_{k\ell}\}$ ; if  $T_{k\ell} > T_{\text{curr\_max}}$ , set  $\text{curr\_max} = (k, \ell)$ .

[Wei, Naik, Harrow, JDT, PRD 2020]



# Quantum Search for Thrust

Grover search to find optimal partition



T  
Grover over  
 $N^2$  partitions  
in  $O(N)$

1. Randomly sample  $i, j \in [N]$
2. Compute  $\vec{p}_i, \vec{p}_j$  via LOOKUP
3. Set  $\vec{r}_{ij} = (\vec{p}_i \times \vec{p}_j) / |\vec{p}_i \times \vec{p}_j|$
4. While  $|\langle \vec{r}_{ij}, \vec{n} \rangle| > \epsilon$ :
  - (a) Let  $\mu = \langle \vec{r}_{ij}, \vec{n} \rangle$
  3. Apply SU( $\mu$ )
  4. Calculate  $\vec{P}_{ij}$
  5. Uncompute SU( $\mu$ )
  - C. Uncompute SU( $\mu$ )
  - D. Reflect  $\vec{r}_{ij}$  across  $\vec{n}$
  - v. Measure the  $\{i, j, T_{ij}\}$
- (b) Let  $\text{max\_it} = \mu$
5. Measure the  $\{i, j, T_{ij}\}$

**Subroutine COMP\_T:**

$$|i\rangle |j\rangle |\vec{0}\rangle |\vec{0}\rangle |\hat{0}\rangle |\vec{0}\rangle |0\rangle \mapsto |i\rangle |j\rangle |\vec{p}_i\rangle |\vec{p}_j\rangle |\hat{0}\rangle |\vec{0}\rangle |0\rangle.$$

I And this?

momentum  $\vec{P}_{ij}$ :

## Looking up classical data

$$U_{\text{LOOKUP}} |i\rangle |\vec{0}\rangle = |i\rangle |\vec{p}_i\rangle$$

## Without qRAM: $O(N)$

[With qRAM:  $O(1)$ , Giovannetti, Lloyd, Maccone, [PRL 2008](#)]

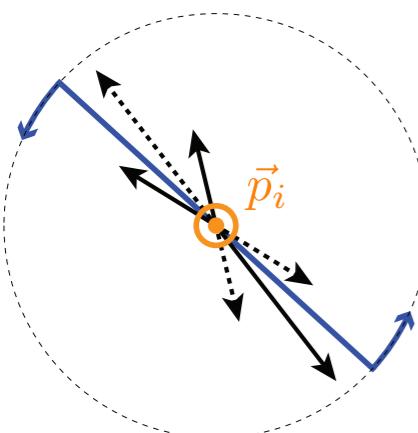


[Wei, Naik, Harrow, JDT, [PRD 2020](#)]

# Final Scorecard for Quantum Thrust

Quantum search gives  $O(N^2) \ll O(N^3)!$

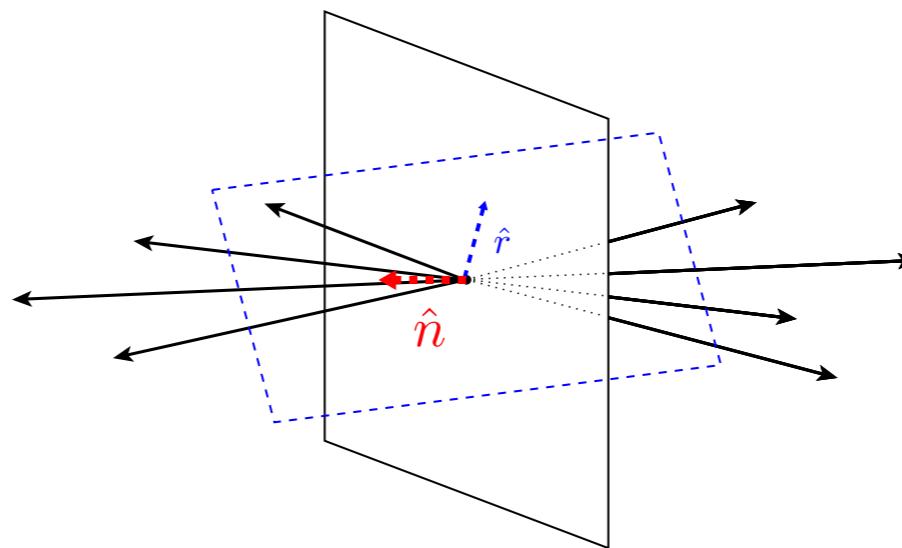
Implementation	Time Usage	Qubit Usage
Classical [2]	$O(N^3)$	—
Classical with Sort (using [3])	$O(N^2 \log N)$	←
Classical with Parallel Sort	$O(N \log N)$	—
Quantum Annealing	Gap Dependent	$O(N)$
Quantum Search: Sequential Model	$O(N^2)$	$O(\log N)$
Quantum Search: Parallel Model	$O(N \log N)$	$O(N \log N)$



But we found new  $O(N^2 \log N)$  algorithm using classical sort...

[Wei, Naik, Harrow, JDT, PRD 2020]  
[classical trick based on Salam, Soyez, JHEP 2007]

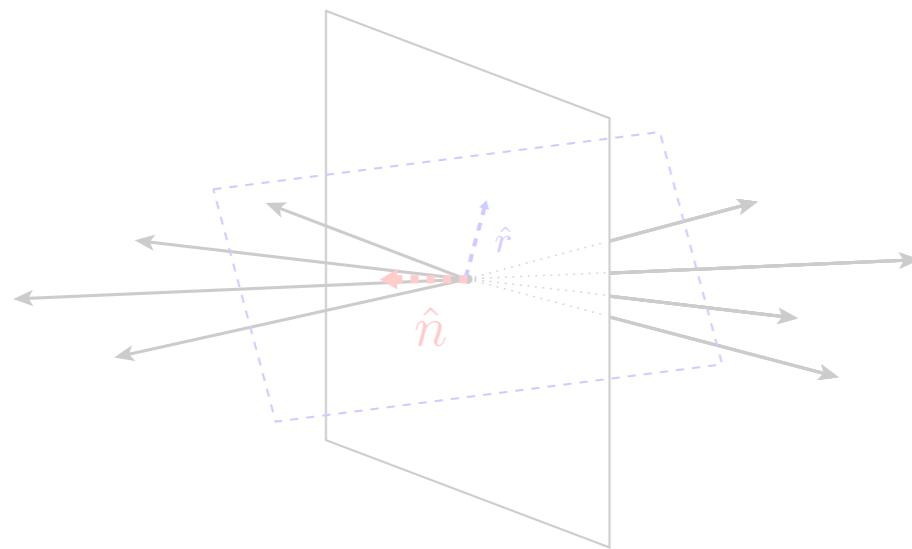




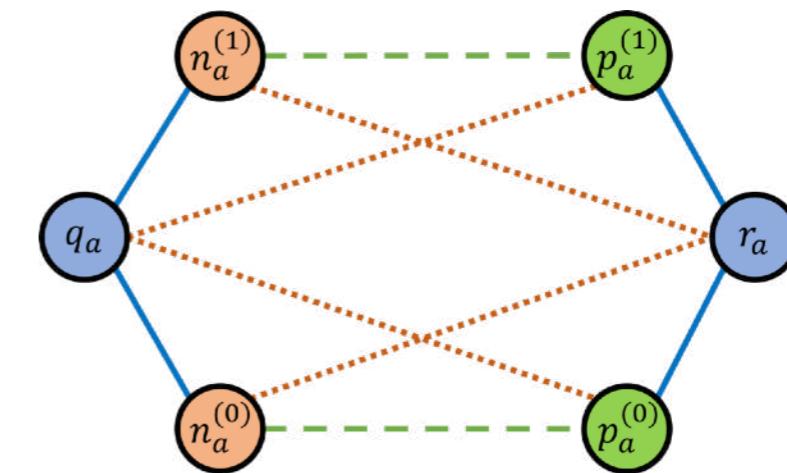
**Quantum Inspiration:**  
*Solving jet optimization using annealing or Grover search*

**Classical Development:**  
*Improved  $O(N^2 \log N)$  thrust algorithm with classical sort*

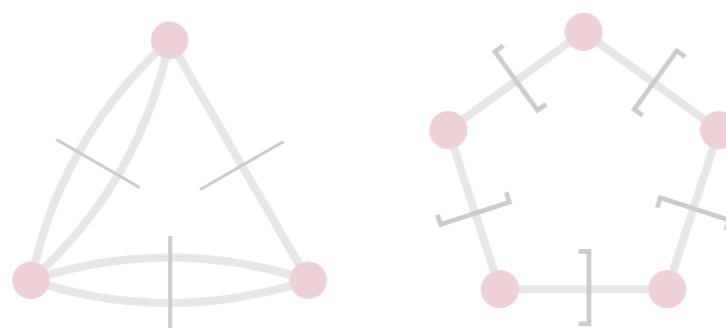
## Challenge of Data Loading



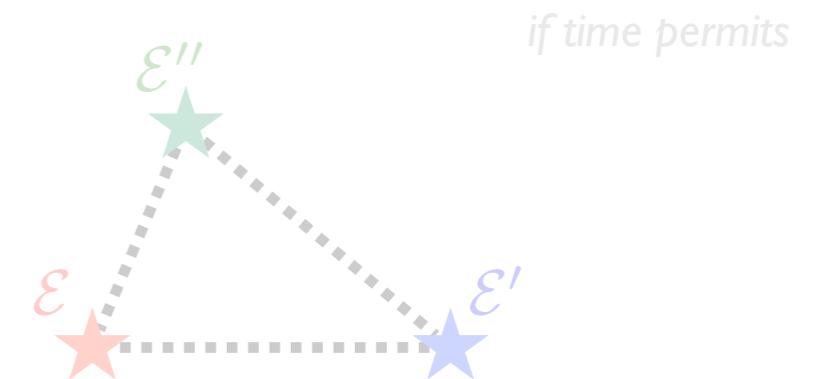
## Degeneracy Engineering



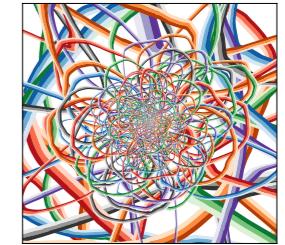
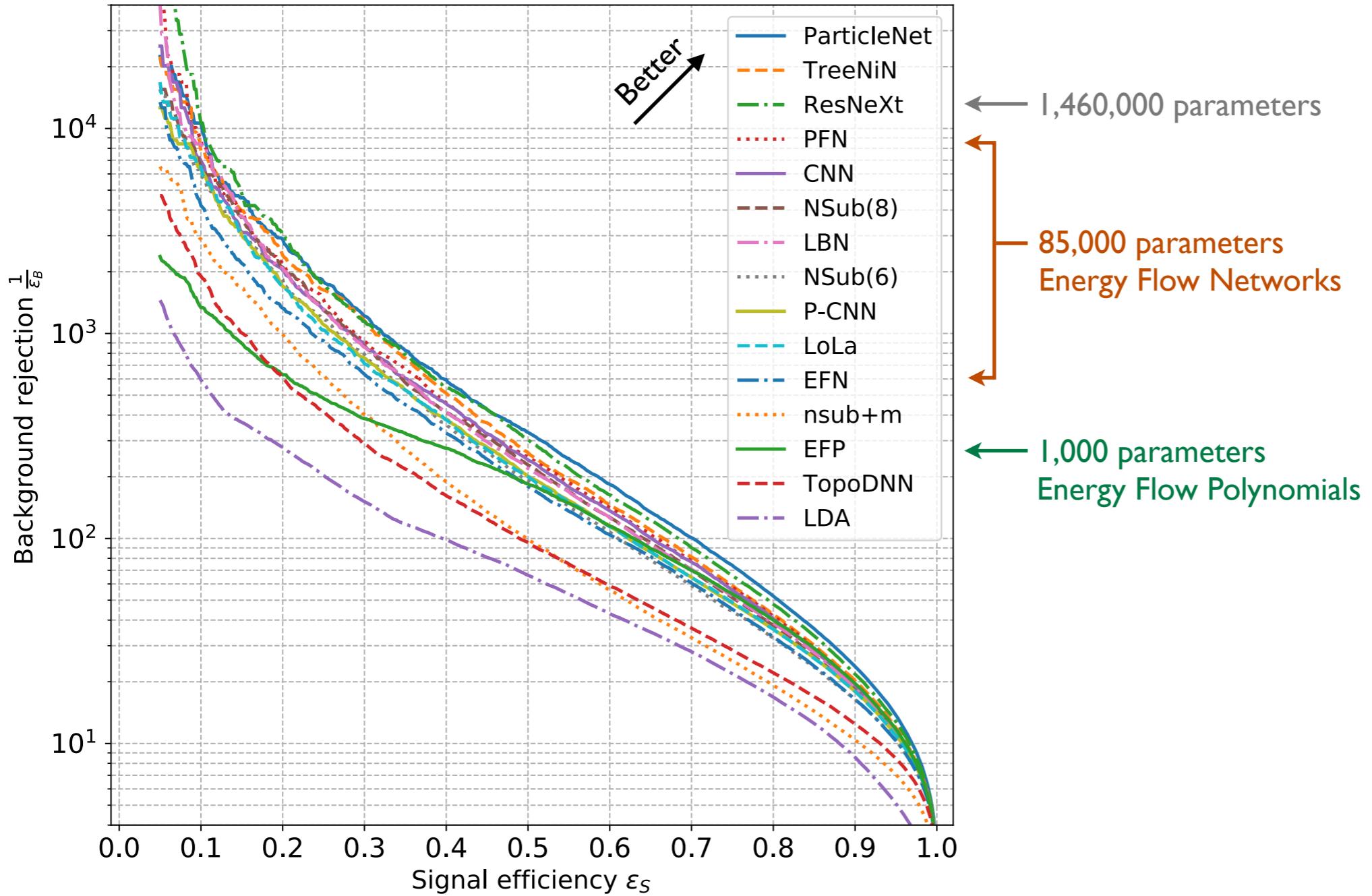
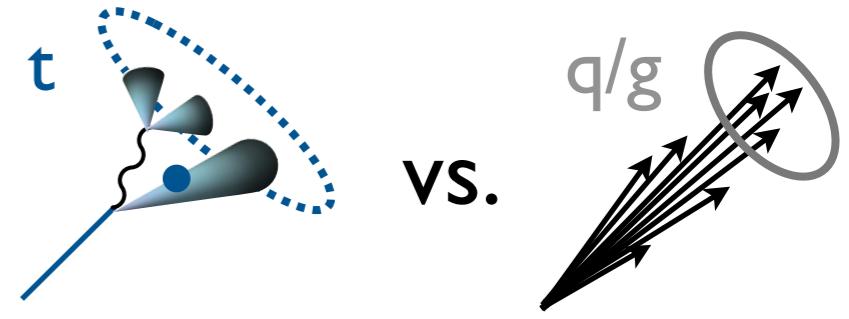
## Superposition for Graphs



## Optimal Transport



# Rise of the Machines?



[Kasieczka, Plehn, et al., [SciPost 2019](#)]

[Komiske, Metodiev, [JDT, JHEP 2018](#); Komiske, Metodiev, [JDT, JHEP 2019](#)]

[LHC baseline based on [JDT, Van Tilburg, JHEP 2011, JHEP 2012](#)]



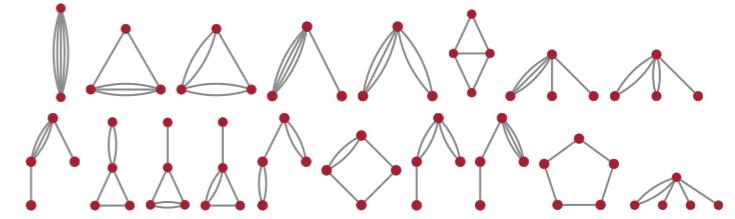
# Energy Flow Polynomials for Jet Substructure

Case study for sparse linear regression

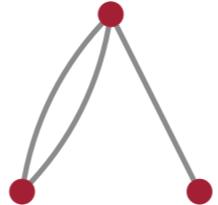
Linear basis for IRC-safe  
collider observables:

(more about IRC safety later)

$$\mathcal{S} = \sum_G s_G \text{EFP}_G$$



e.g.


$$= \sum_{i_1=1}^M \sum_{i_2=1}^M \sum_{i_3=1}^M z_{i_1} z_{i_2} z_{i_3} \theta_{i_1 i_2}^2 \theta_{i_1 i_3}$$

Very powerful statement... except **thousands of terms needed**

(still better than deep learning!)

Regularization?

L<sub>2</sub>-Norm (Ridge): Not sparse

L<sub>1</sub>-Norm (Lasso): Biased answers

L<sub>0</sub>-Norm: NP-hard  $\Rightarrow$  Annealing?

[Komiske, Metodiev, JDT, JHEP 2018]



# Sparse Linear Regression

**Standard Loss Function**

$$L_{\text{MSE}} = \sum_{s \in \mathcal{S}} \left( y_s - h(\vec{x}_s) \right)^2$$

**Standard Linear Regression**

$$h(\vec{x}; \{c_a\}) = \sum_{a=1}^K c_a h_a(\vec{x})$$

**Standard Binary Encoding**

$$c_a = \sum_{i=1}^M g_i b_a^{(i)}$$

**Standard Regularization**

$$L = L_{\text{MSE}} + \lambda R$$

**Standard p-Norm Penalty**

$$R^{(p)} = \sum_{a=1}^K |c_a|^p$$

*L<sub>0</sub>-Norm ( $p = 0$ )  
not of quadratic form  
(i.e. Ising/QUBO)...*

# Sparse Linear Regression for Annealing

Standard Loss Function

$$L_{\text{MSE}} = \sum_{s \in \mathcal{S}} \left( y_s - h(\vec{x}_s) \right)^2$$

Standard Linear Regression

$$h(\vec{x}; \{c_a\}) = \sum_{a=1}^K c_a h_a(\vec{x})$$

Standard Binary Encoding

$$c_a = \sum_{i=1}^M g_i b_a^{(i)}$$

Standard Regularization

$$L = L_{\text{MSE}} + \lambda R$$

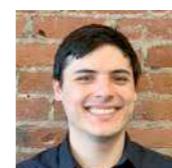
Effective 0-Norm Penalty

$$R_a^{(0-\text{control})} = r_a + (1 - r_a) \sum_{i=1}^M b_a^{(i)}$$

PRELIMINARY

Key: Use a *latent bit* to “quadratic-ify”  $L_0$  loss function

[Anschuetz, Funcke, Komiske, Kryhin, JDT, in progress]



# Sparse Linear Regression for Efficient Annealing

## Standard Loss Function

$$L_{\text{MSE}} = \sum_{s \in \mathcal{S}} \left( y_s - h(\vec{x}_s) \right)^2$$

## Standard Linear Regression

$$h(\vec{x}; \{c_a\}) = \sum_{a=1}^K c_a h_a(\vec{x})$$

## Redundant Binary Encoding

$$c_a = \sum_{i=1}^M g_i (p_a^{(i)} - n_a^{(i)})$$

## Standard Regularization

$$L = L_{\text{MSE}} + \lambda R$$

## Efficient 0-Norm Penalty

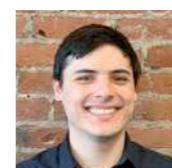
$$R_a^{(0-\text{paired})} = q_a + (1 - q_a + 2r_a) \sum_{i=1}^M p_a^{(i)}$$

PRELIMINARY

Key: *Degeneracy Engineering*

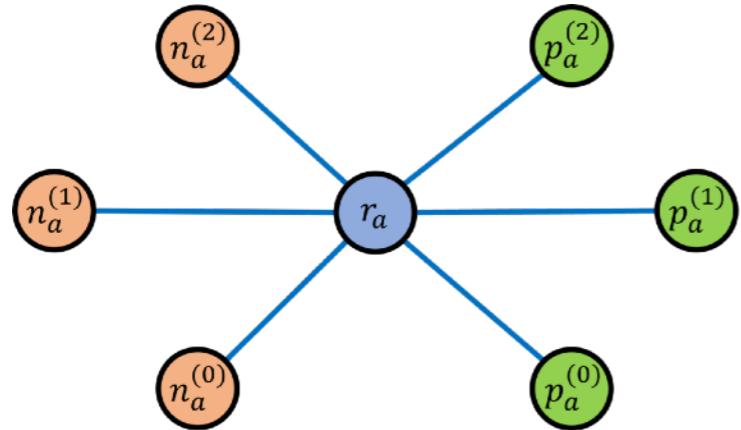
$$+ r_a + (1 - r_a + 2q_a) \sum_{i=1}^M n_a^{(i)} - 2 \sum_{i=1}^M p_a^{(i)} n_a^{(i)}$$

[Anschuetz, Funcke, Komiske, Kryhin, JDT, in progress]



# Degeneracy Engineering

Single Latent Bit



Irrelevant Excited States



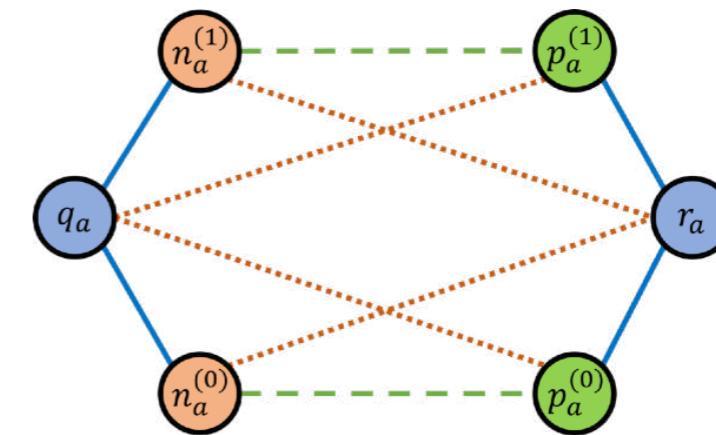
Degenerate Excited State



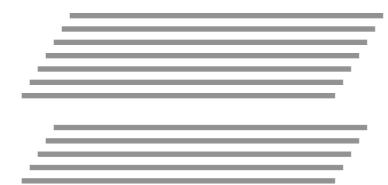
Ground State



Double Latent Bit



(More) Irrelevant Excited States



(More) Degenerate Excited State

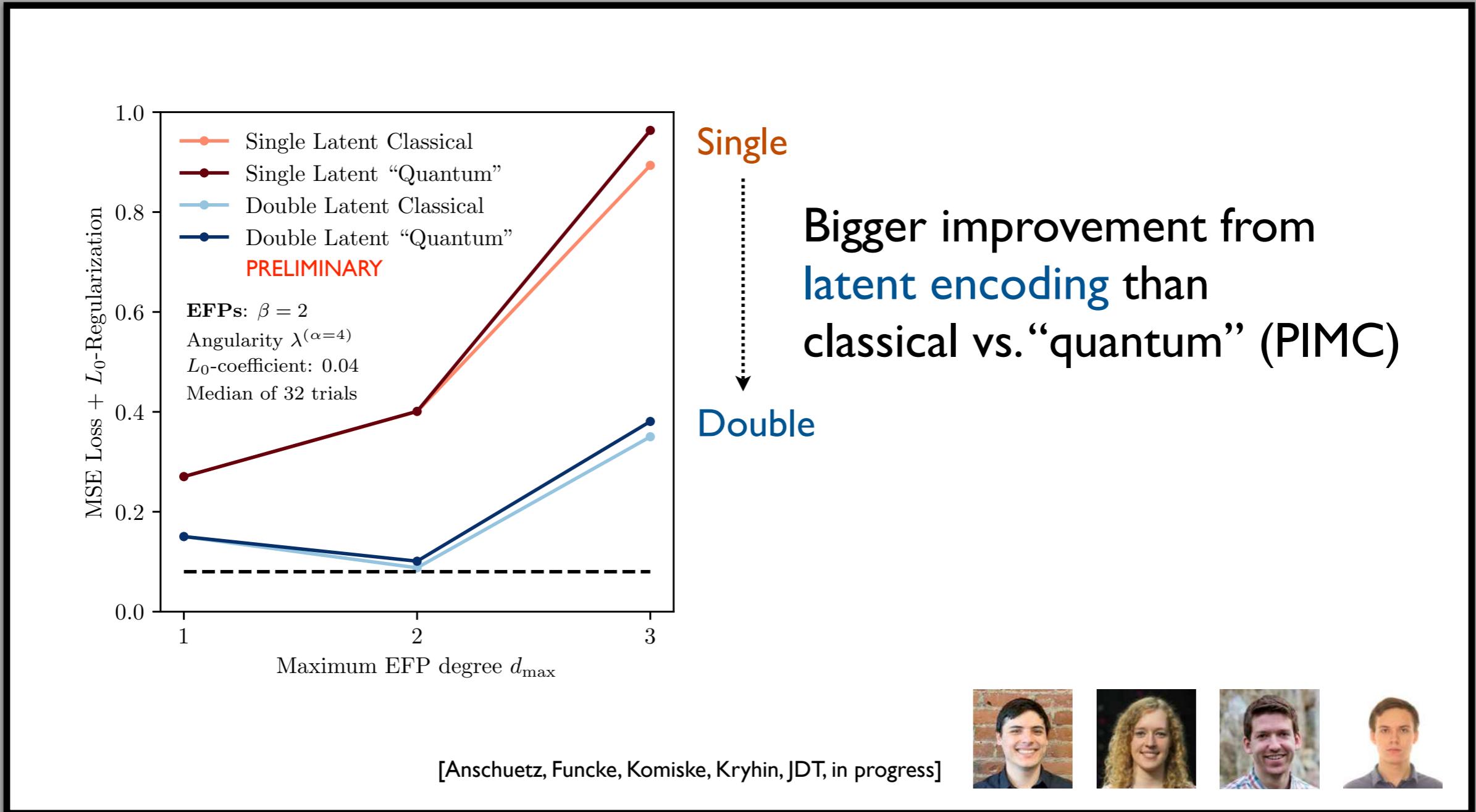


Degenerate Ground State

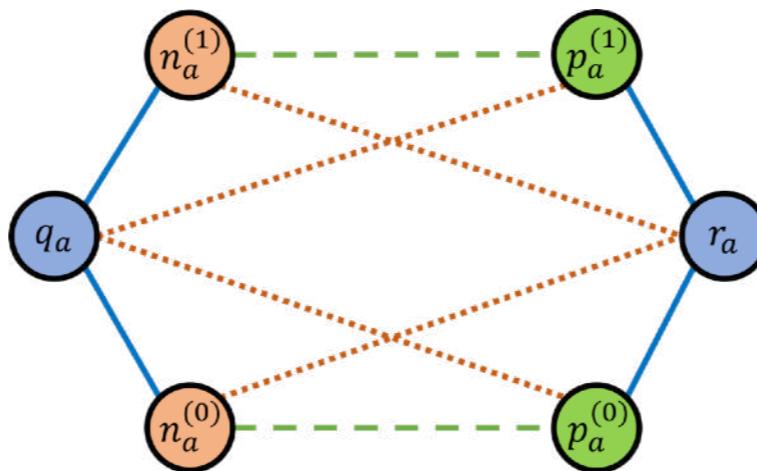


*More efficient as relative degeneracy of ground state increases*

# Degeneracy Engineering



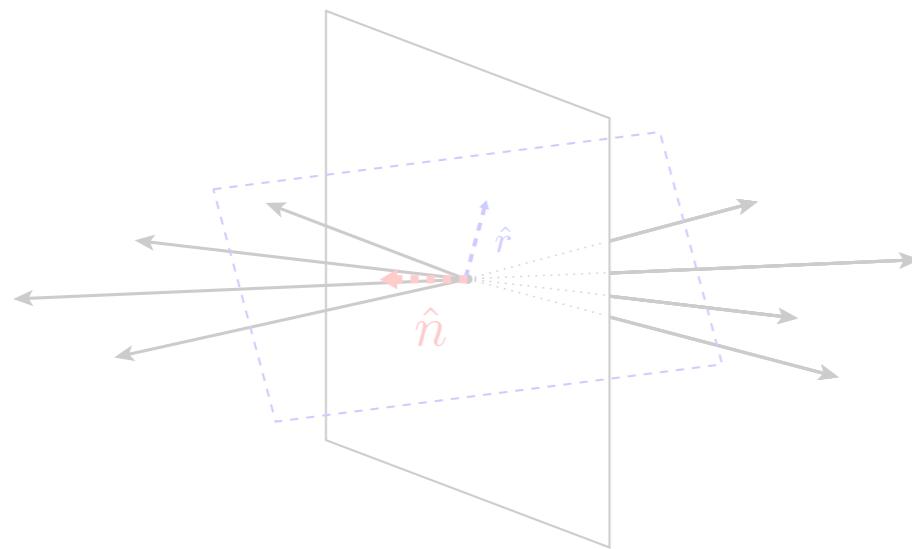
*More efficient as relative degeneracy of ground state increases*



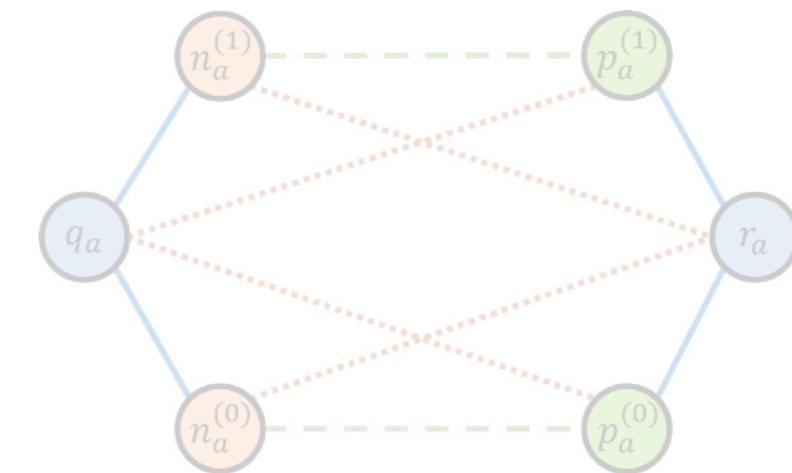
**Quantum Inspiration:**  
*Finding sparse regression solutions through annealing*

**Classical Development:**  
*Improved quadratic loss landscape for L<sub>0</sub>-norm regularization*

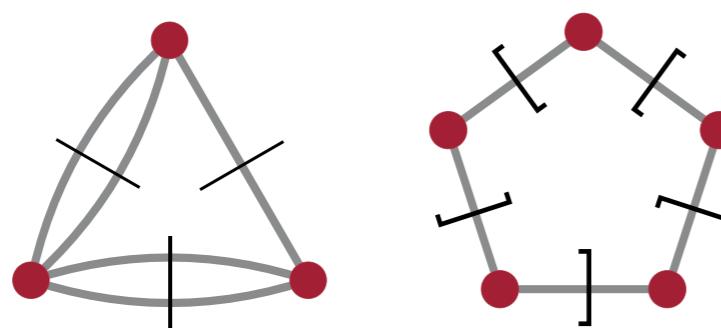
## Challenge of Data Loading



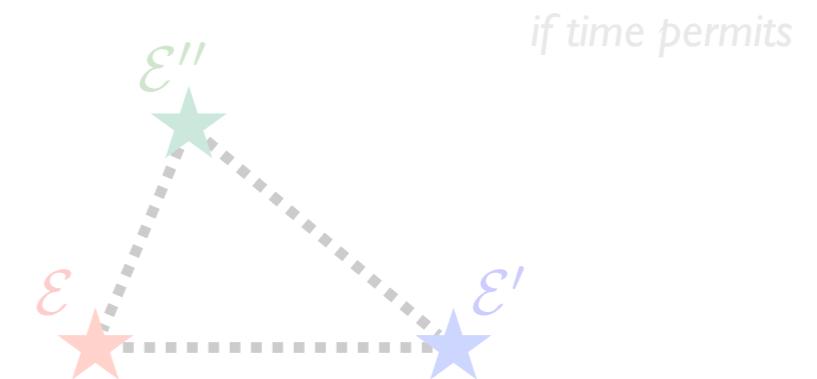
## Degeneracy Engineering



## Superposition for Graphs

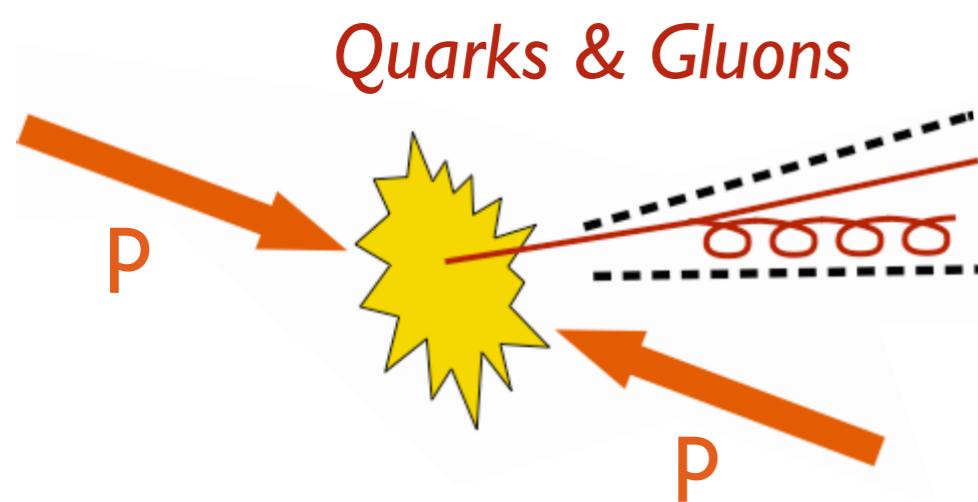


## Optimal Transport



# Energy Flow Representation

Respects *infrared and collinear safety*

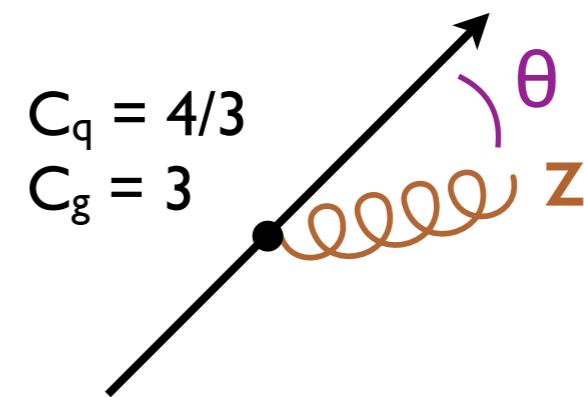


Conceptual challenge:  
Splitting obscures quantum coherence,  
complicates quantum encoding

Conceptual opportunity:  
**IRC safety** has relevance for  
**quantum chemistry** (see backup)

## Altarelli-Parisi Splitting

Core prediction of **QCD**



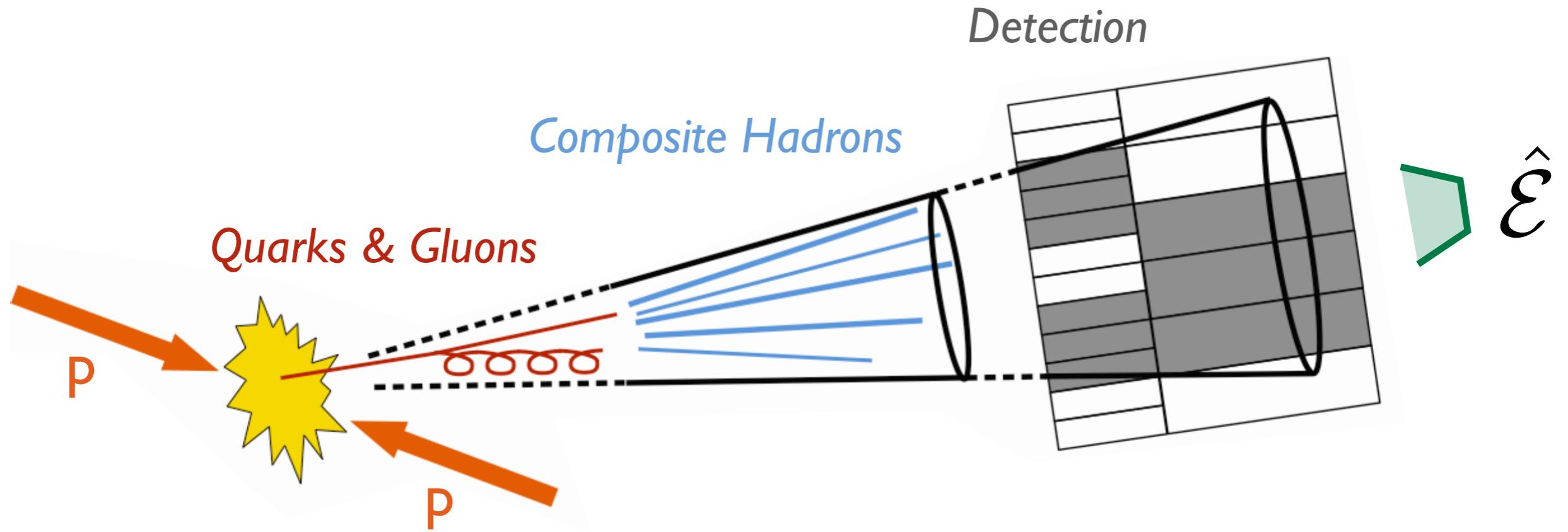
$$dP_{i \rightarrow ig} \simeq \frac{2\alpha_s}{\pi} C_i \frac{d\theta}{\theta} \frac{dz}{z}$$

Collinear   Soft

# Energy Flow Representation

Respects *infrared and collinear safety*

Theory



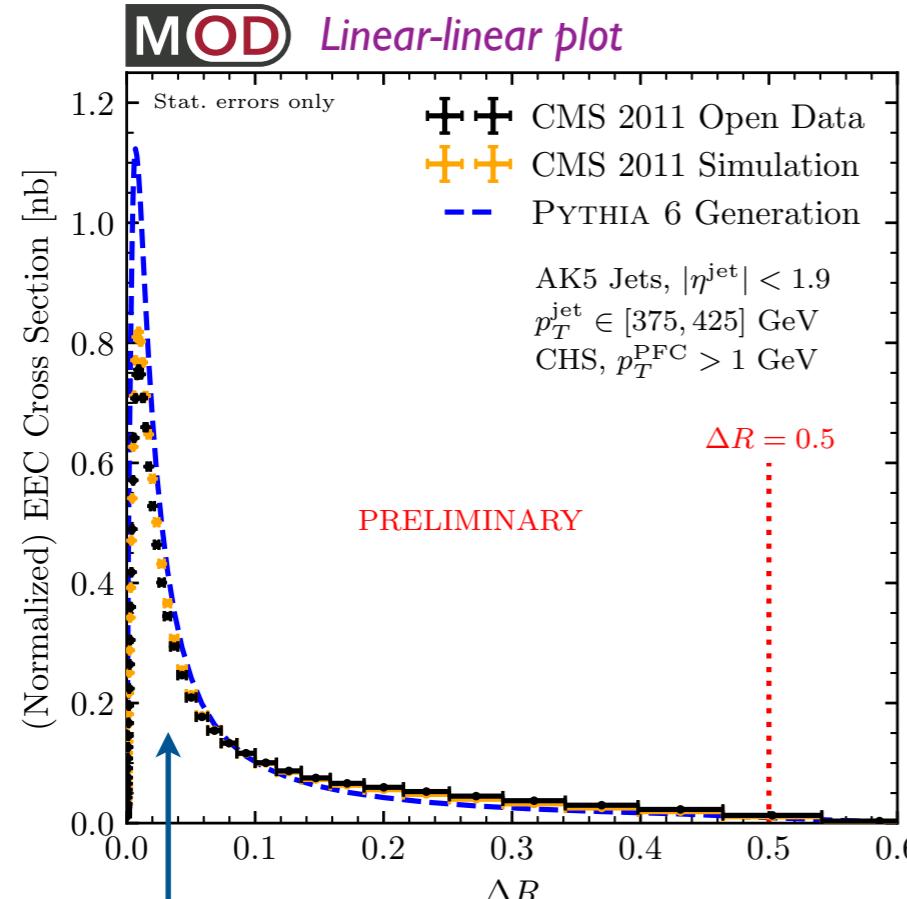
## Energy Flow:

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

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

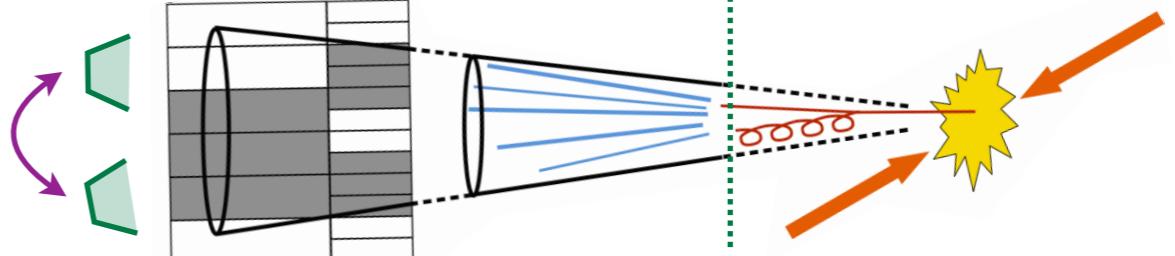
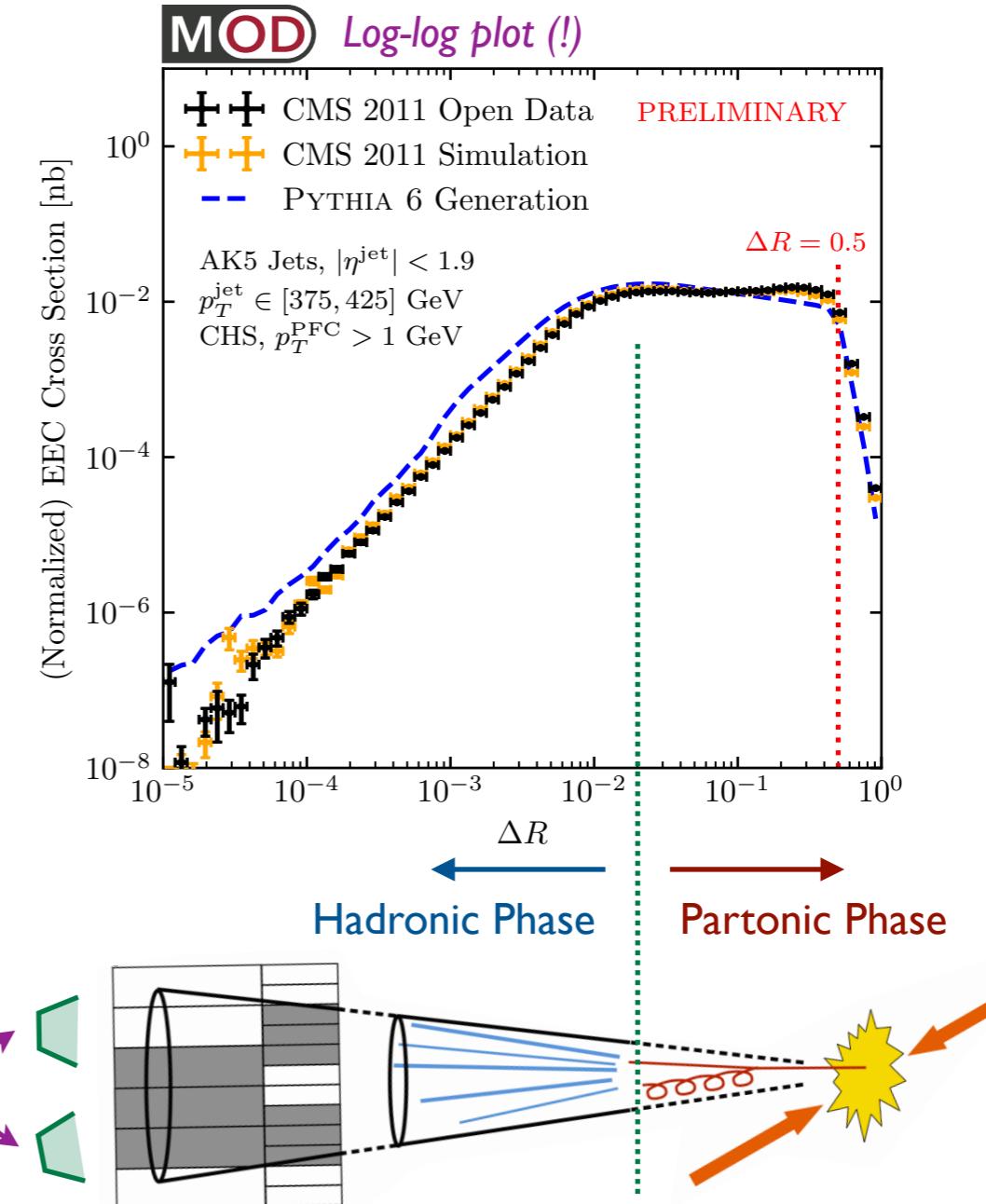
[see e.g. Sveshnikov, Tkachov, [PLB 1996](#); Hofman, Maldacena, [JHEP 2008](#); Mateu, Stewart, [JDT, PRD 2013](#); Belitsky, Hohenegger, Korchemsky, Sokatchev, Zhiboedov, [PRL 2014](#); Chen, Moult, Zhang, Zhu, [PRD 2020](#)]

# QCD Phase Transition in Jets?



Are we learning something about small angle limit of QCD?

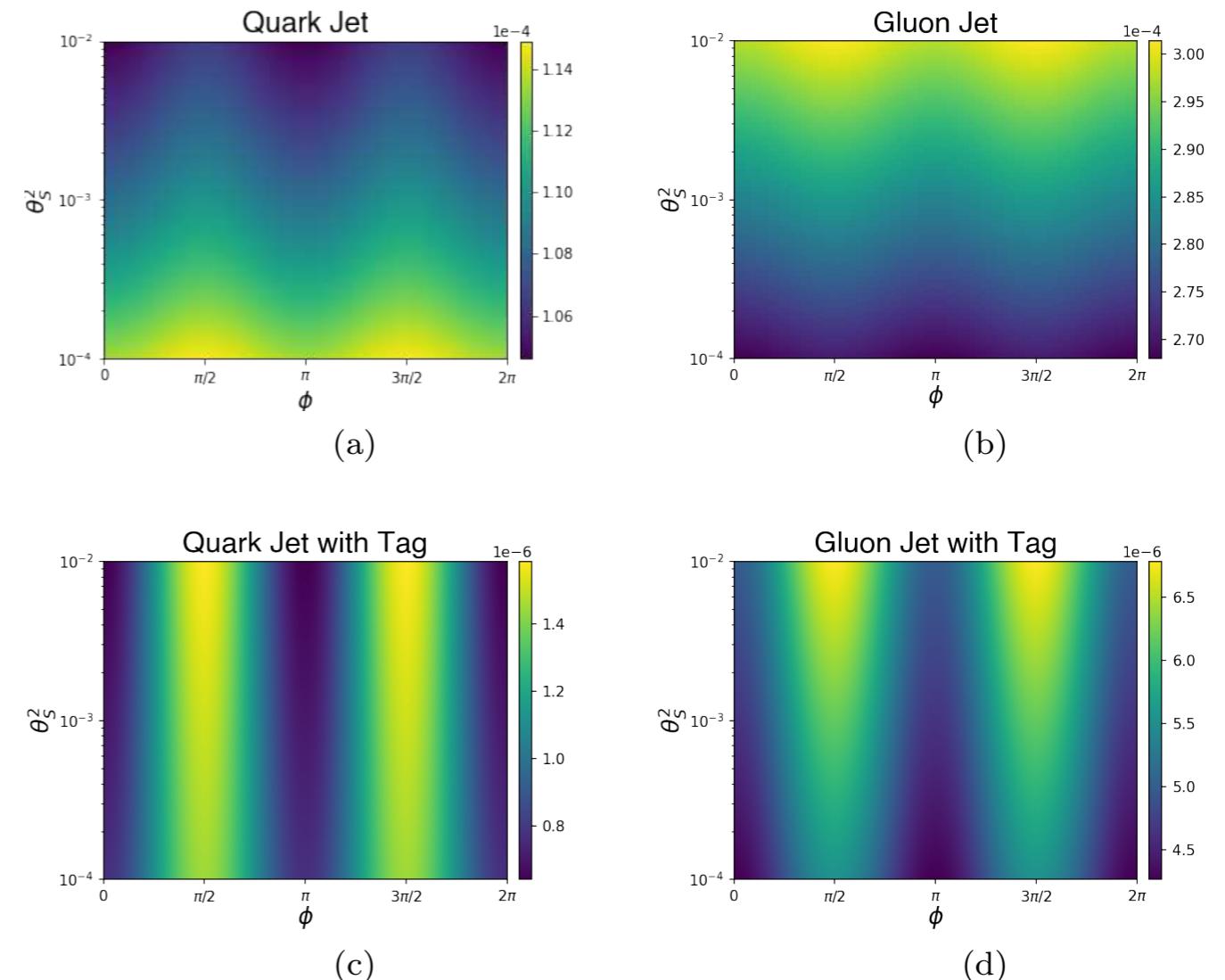
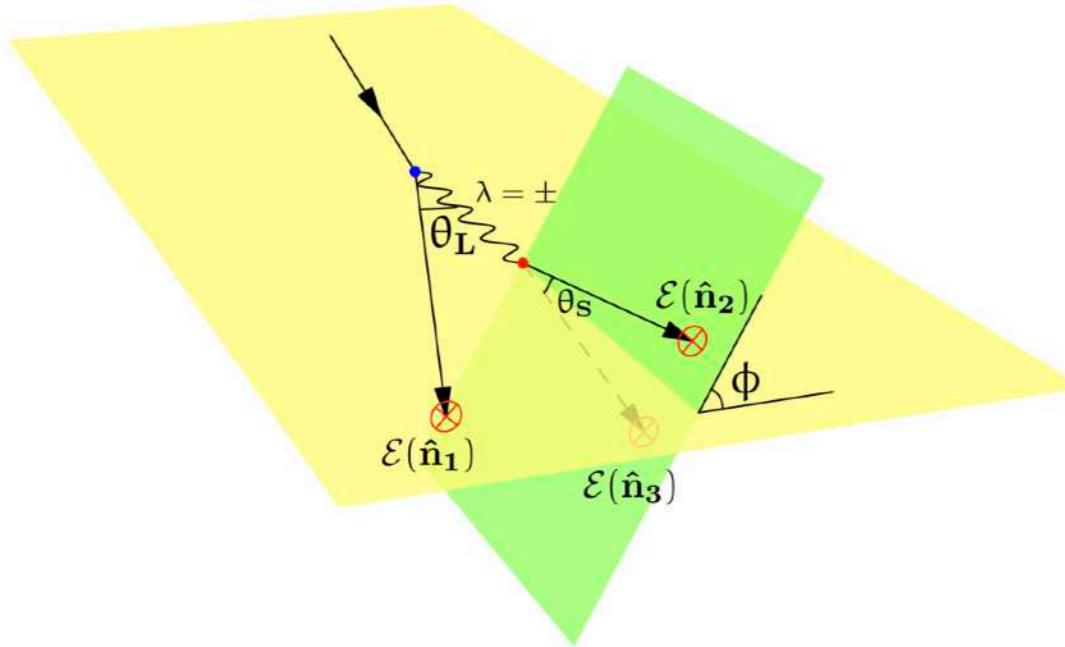
First Jet EEC Plot from the LHC (!)



[Komiske, Moult, JDT, Zhu, in progress; see talks by Moult, [BOOST 2019](#), [BOOST 2020](#)]



# Quantum Fun with Three Point Correlators



(with help from b-tagging)

*Extracting quantum interference effects of spinning gluons!*

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

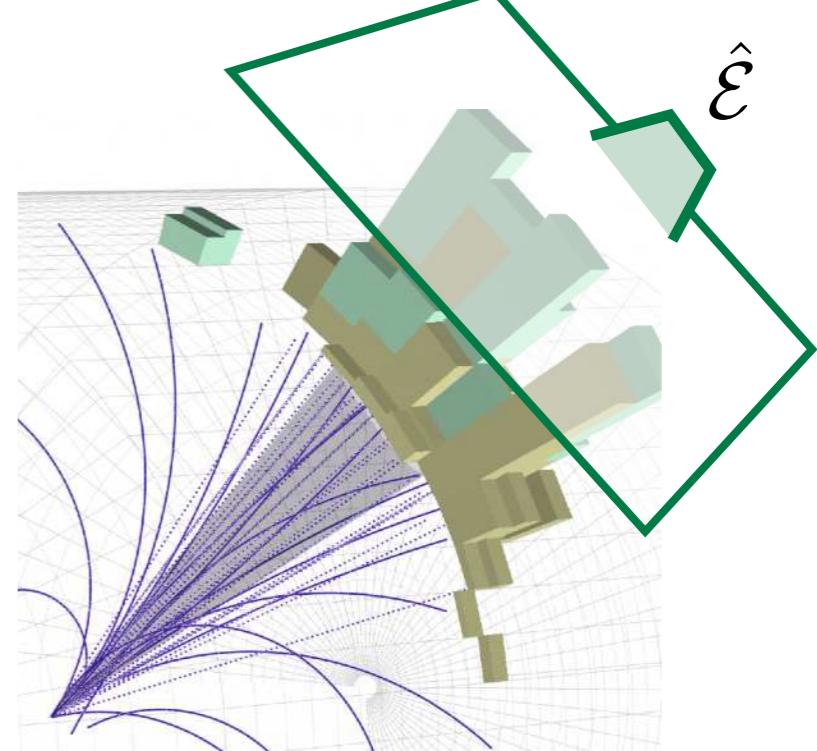
# Jets as Weighted Point Clouds

- Energy-Weighted Directions

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

↑      |  
Energy      Direction

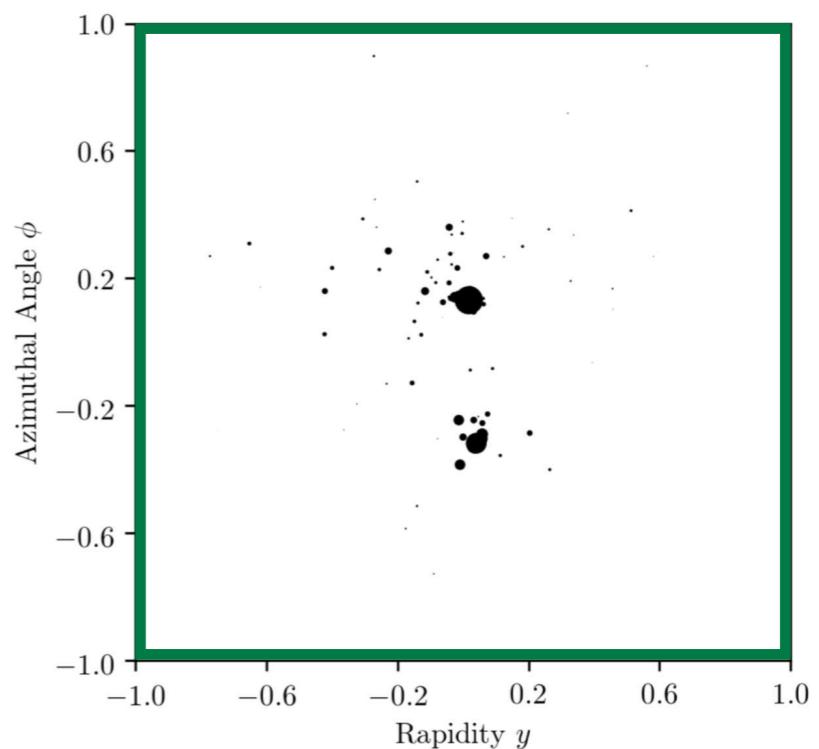
(suppressing “unsafe” charge/flavor information)



- Equivalently: Energy Density

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

↑      ↑  
Energy      Direction



# Quantum Loading of Point Clouds?

**M particles takes  $O(M)$  quantum loading** (w/o qRAM)

$$U_{\text{LOOKUP}} |i\rangle |\vec{0}\rangle = U_{\text{LOOKUP}} |i\rangle |\vec{p}_i\rangle$$

**$M^2$  pairs also takes  $O(M)$  quantum**

$$U_{\text{LOOKUP}} |i\rangle |\vec{0}\rangle |j\rangle |\vec{0}\rangle = U_{\text{LOOKUP}} |i\rangle |\vec{p}_i\rangle |j\rangle |\vec{p}_j\rangle$$

**$M^3$  triplets also takes  $O(M)$  quantum**

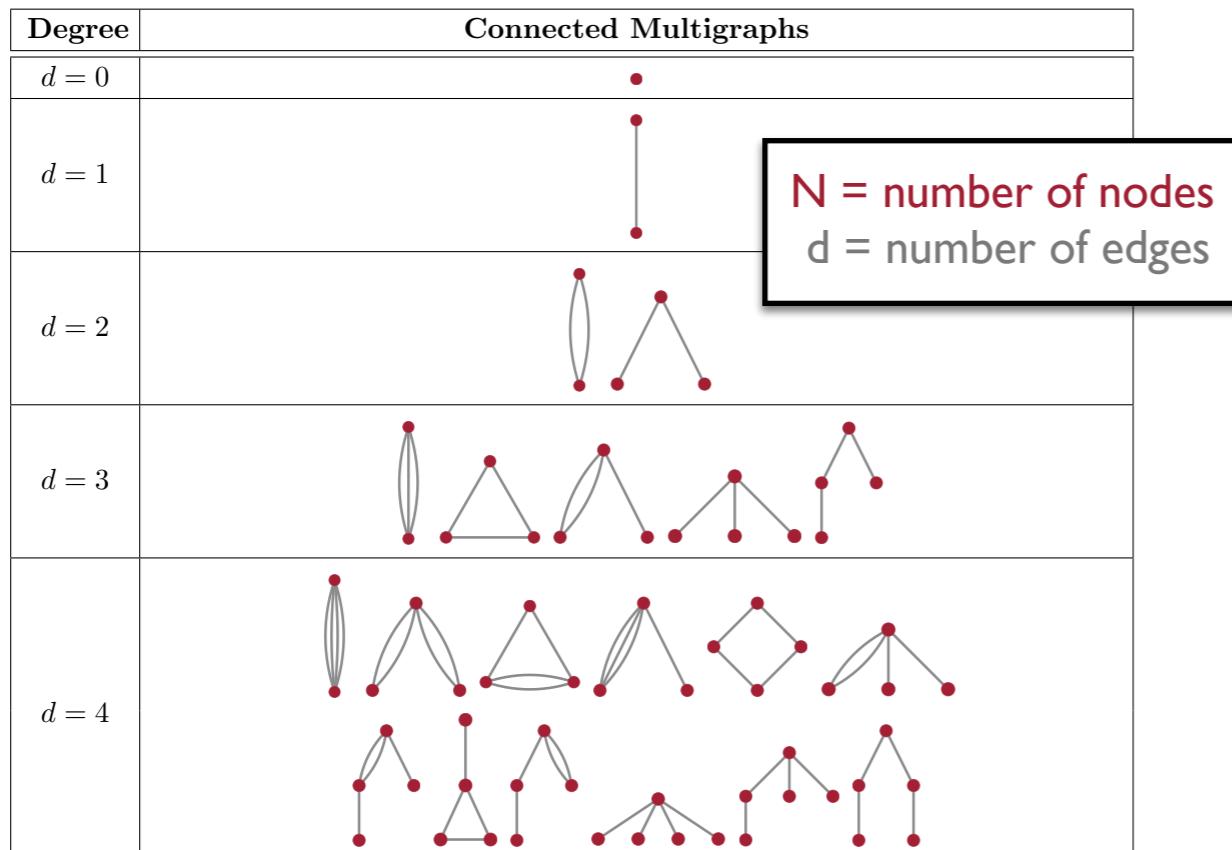
$$U_{\text{LOOKUP}} |i\rangle |\vec{0}\rangle |j\rangle |\vec{0}\rangle |k\rangle |\vec{0}\rangle = U_{\text{LOOKUP}} |i\rangle |\vec{p}_i\rangle |j\rangle |\vec{p}_j\rangle |k\rangle |\vec{p}_k\rangle$$

***Combinatorial loading cheap with quantum superposition***

Sadly, combinatorial processing is still expensive, though speed-ups possible with quantum sampling

# Combinatorics of Energy Flow Polynomials

EFP correlating  $N$ -plets of  
M particles naively costs  $O(M^N)$



Cheaper at small  $d$  with variable elimination

Enumerating EFPs is  
combinatorial challenge

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

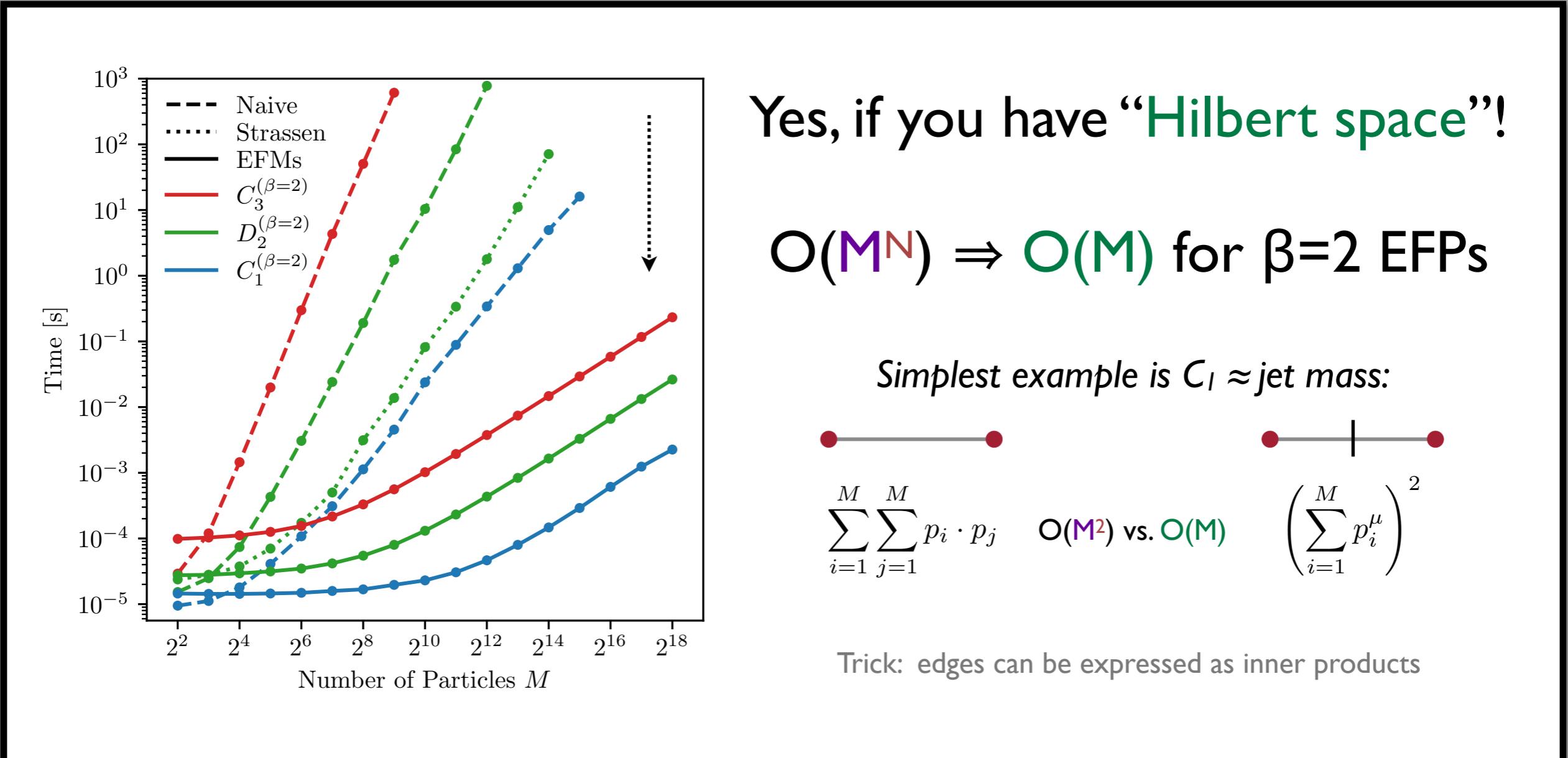
EFPs are generically linearly dependent

Is there *classical analog to quantum superposition?*

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



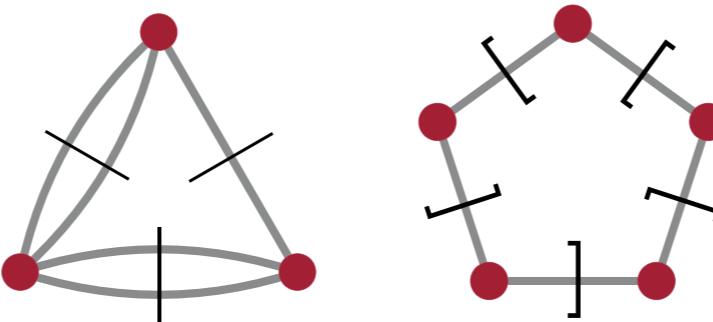
# Combinatorics of Energy Flow Polynomials



Is there *classical analog* to *quantum superposition*?

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

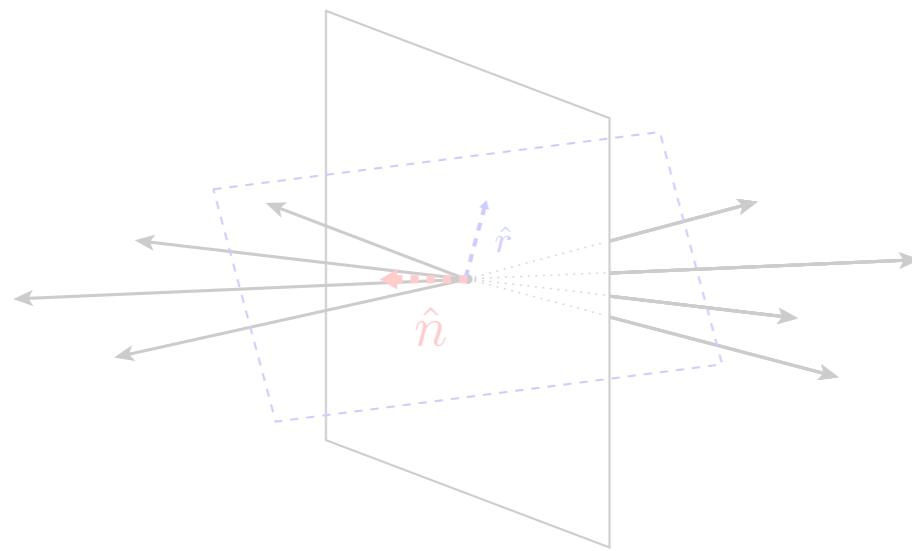




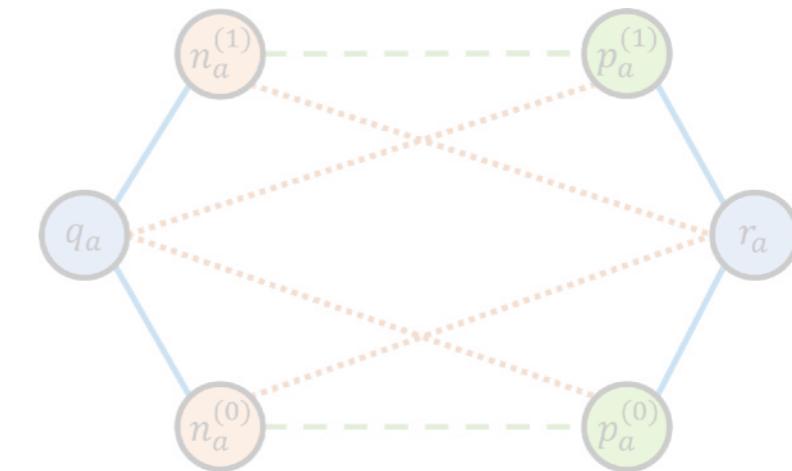
**Quantum Inspiration:**  
*Fast data loading when you can leverage superposition*

**Classical Development:**  
*Blazingly fast computation of jet substructure observables*

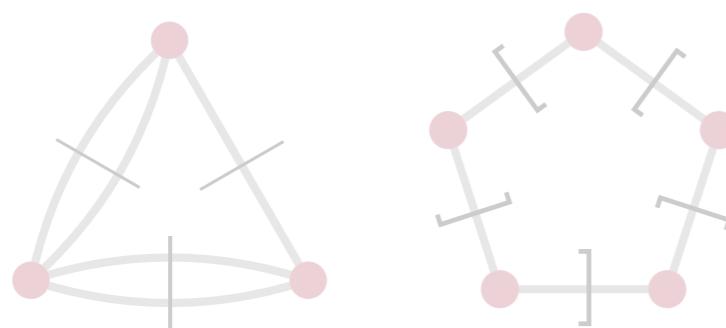
## Challenge of Data Loading



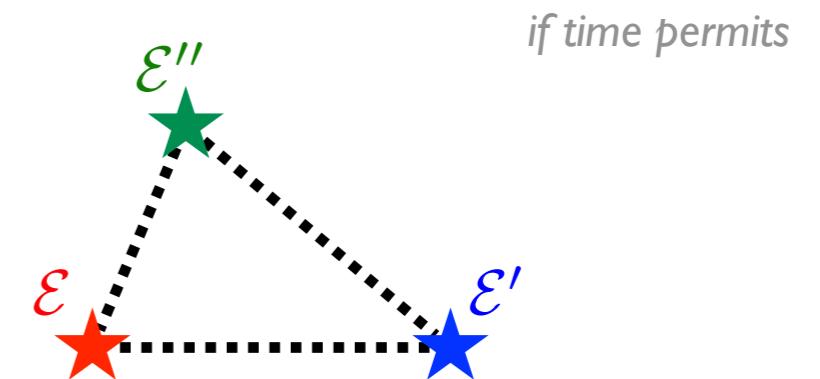
## Degeneracy Engineering



## Superposition for Graphs



## Optimal Transport



# How Big Can We Dream?

*What if we abandon classical efficiency, hoping for future quantum advances?*

I'm not ready to dream of exponentially hard problems...

...but I am ready to look beyond  $O(N_{\text{event}})$  histograms!

**Disclaimer: Original motivation was different**

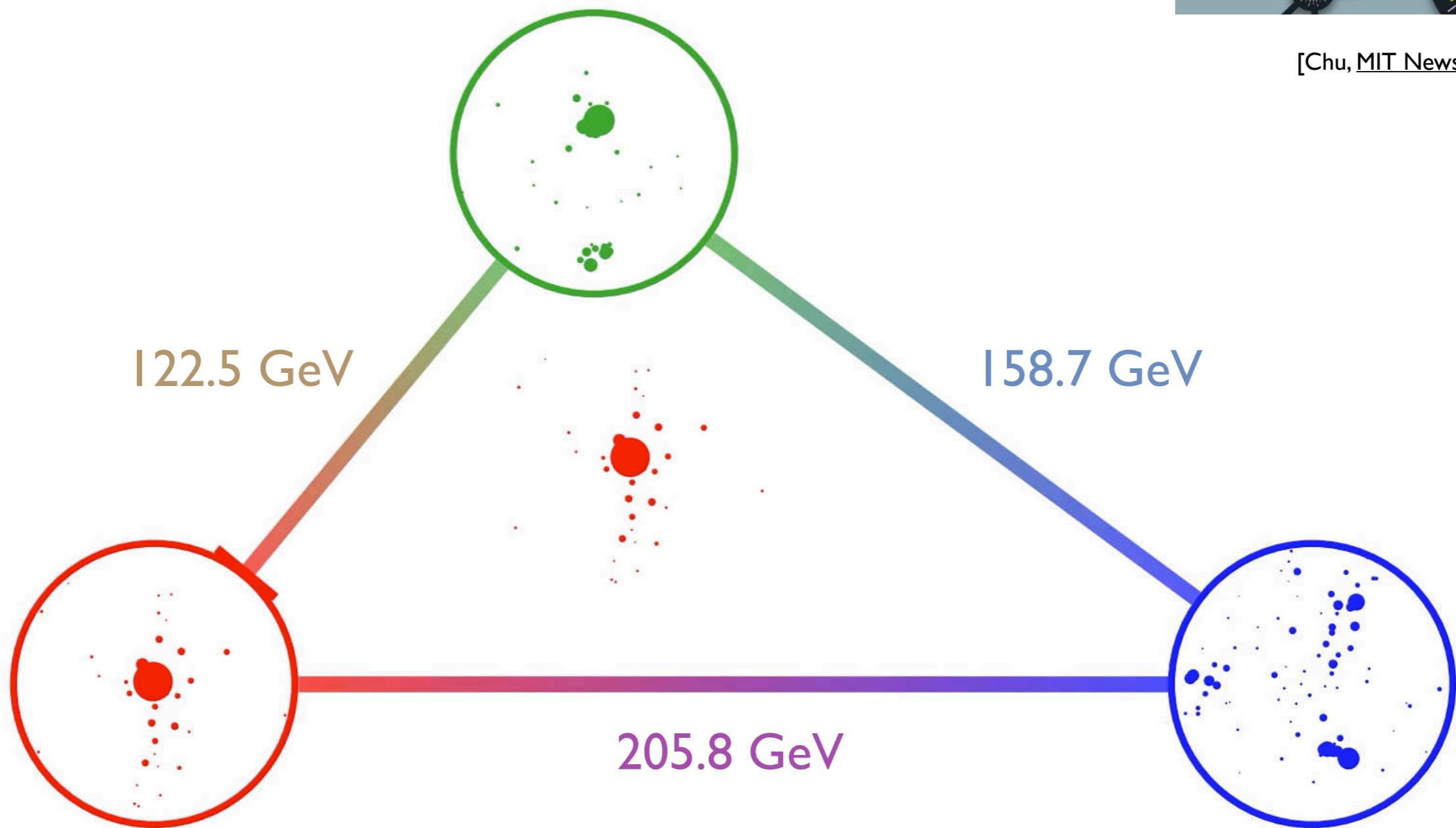
*How can we compress classical data so it fits on near-term quantum devices?*

# Graph of $O(N^2)$ Event Pairs

Inspired by Earth Mover's Distance (a.k.a. Wasserstein metric)



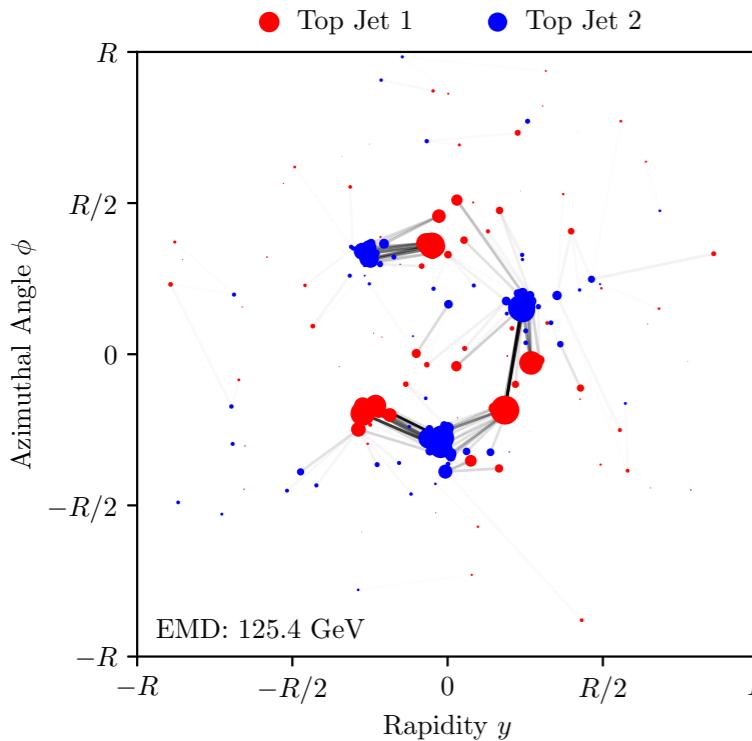
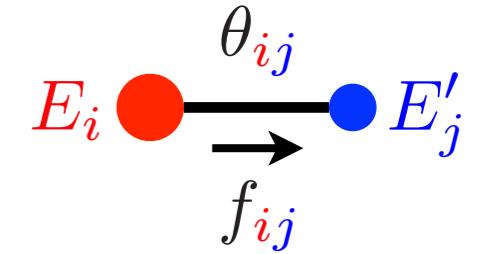
[Chu, MIT News July 2019]



[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](#)]  
[EMD in Monge, 1781; Kantorovich, 1939; Vaserštejn, 1969; Peleg, Werman, Rom, [IEEE 1989](#); Rubner, Tomasi, Guibas, [ICCV 1998](#), [ICJV 2000](#)]



# The Energy Mover's Distance

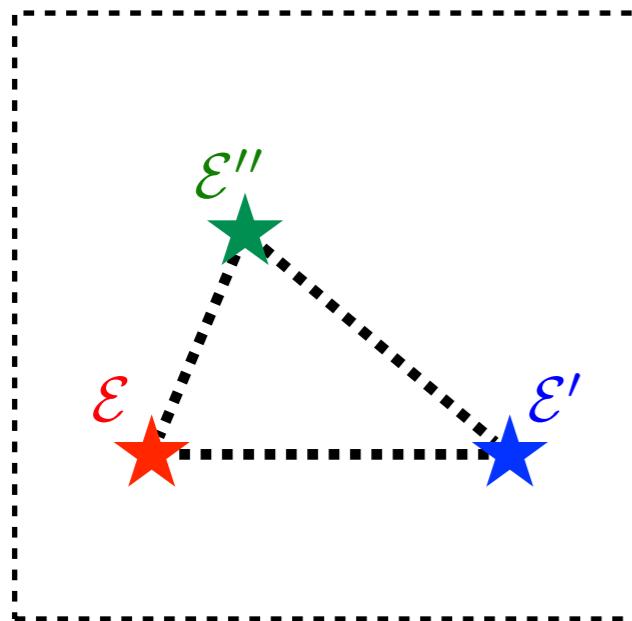


Optimal transport between energy flows...

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

↑  
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)

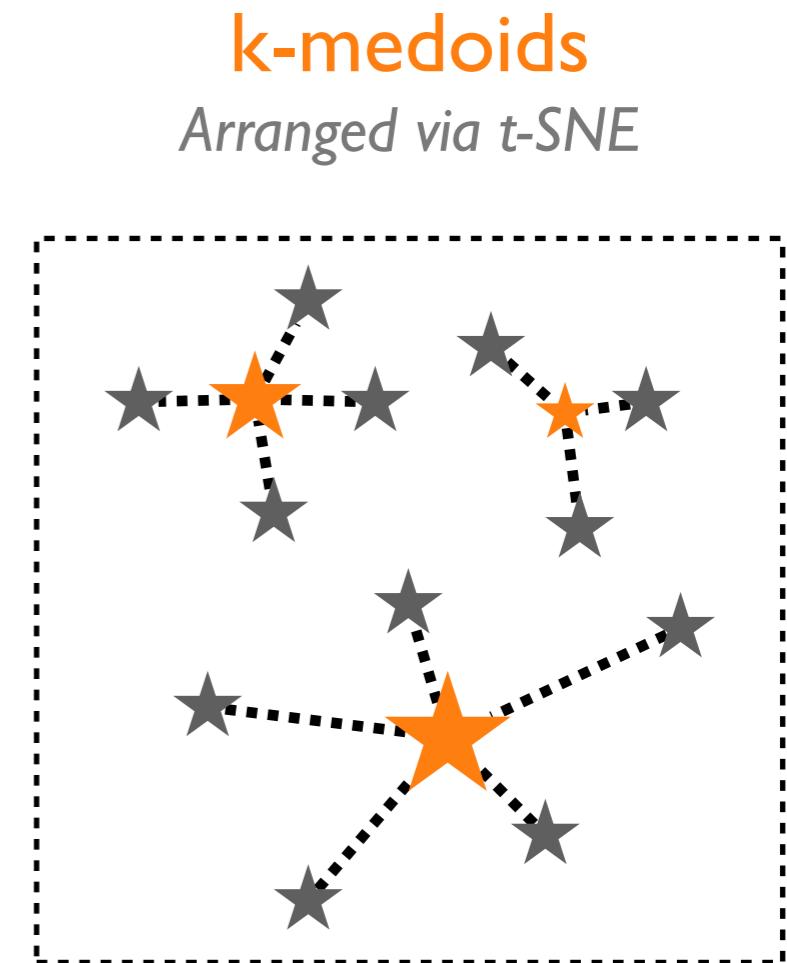
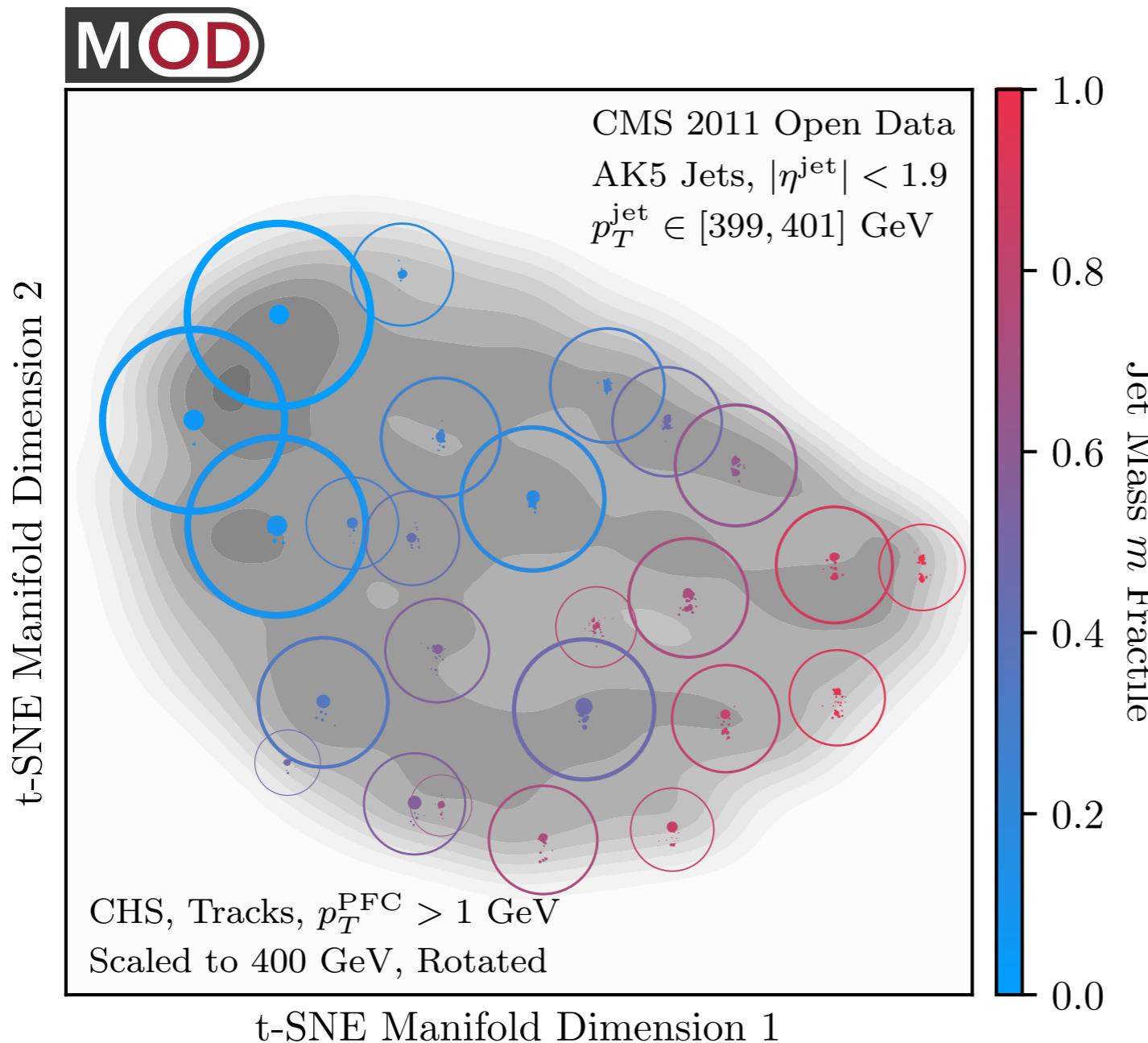
[Komiske, Metodiev, JDT, [PRL 2019](#)  
 [see also Pele, Werman, [ECCV 2008](#); Pele, Taskar, [GSI 2013](#)]  
 [see flavored variant in Crispim Romão, Castro, Milhano, Pedro, Vale, [EPJC 2021](#)]  
 [see computational speed up in Cai, Cheng, Craig, [PRD 2020](#)]



# Most Representative Jets



[<http://opendata.cern.ch/>]



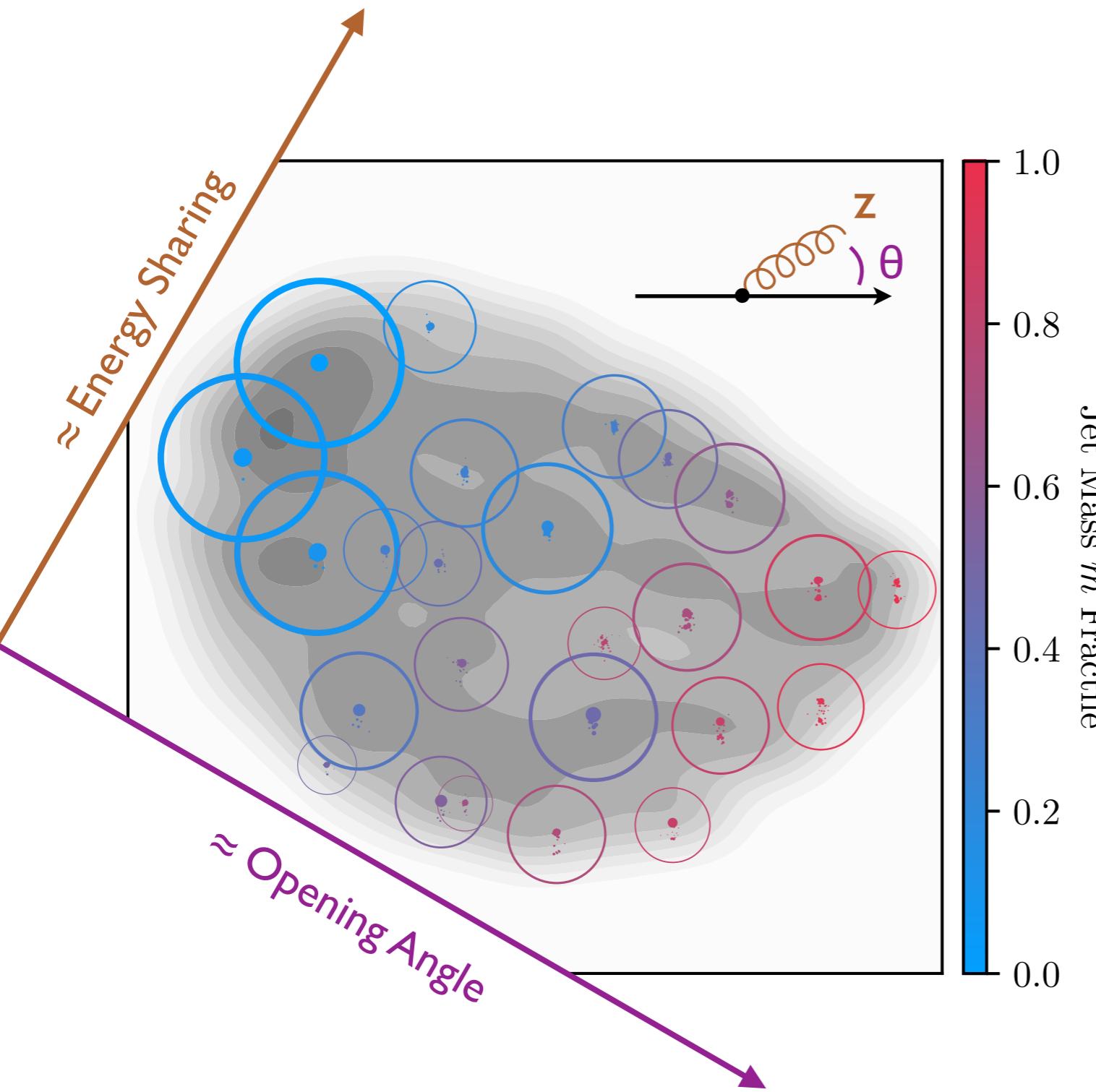
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020]  
[using van der Maaten, Hinton, JMLR 2008; using CMS Open Data]



# Most Representative Jets



[<http://opendata.cern.ch/>]



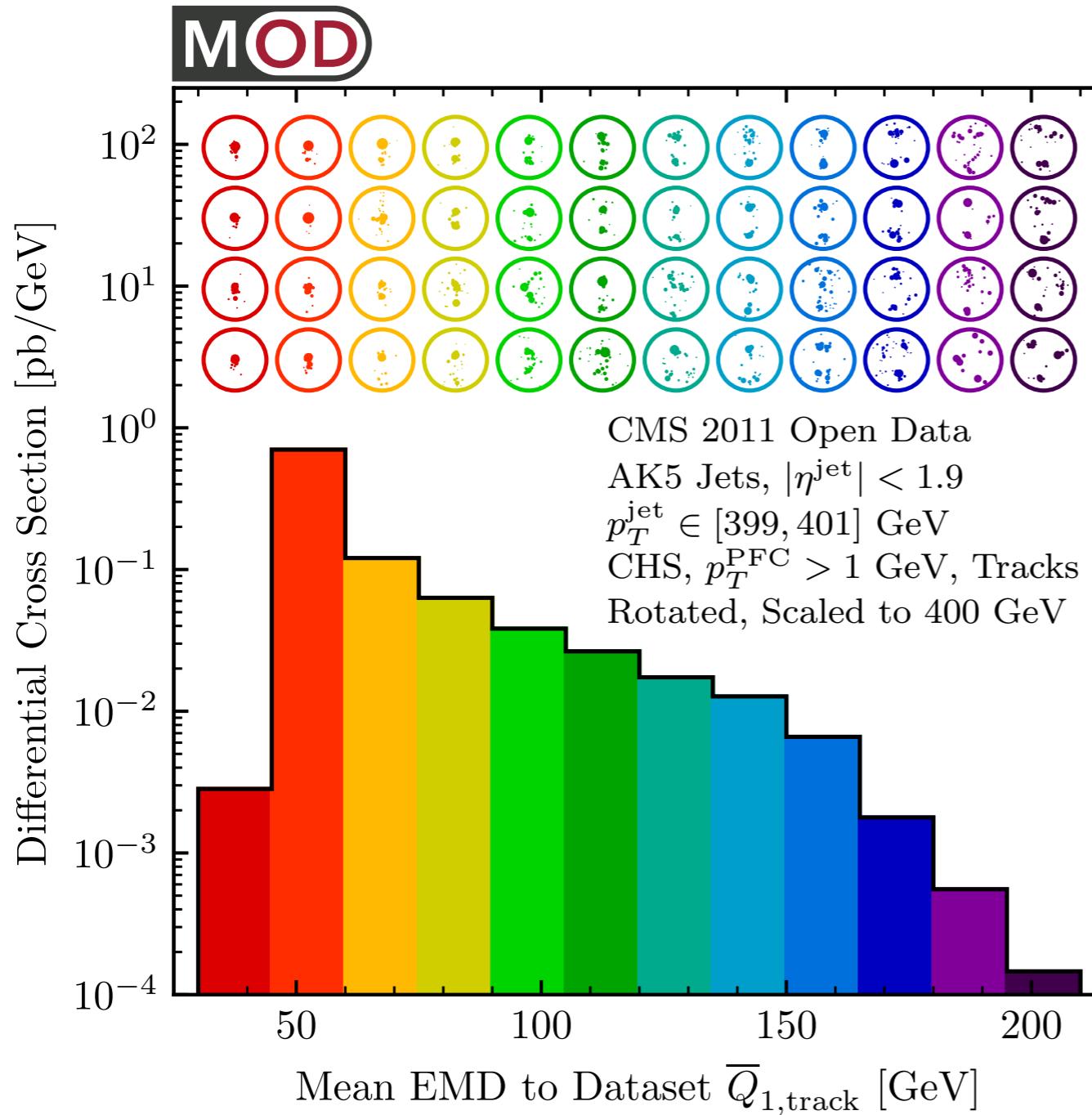
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020]  
[using van der Maaten, Hinton, JMLR 2008; using CMS Open Data]



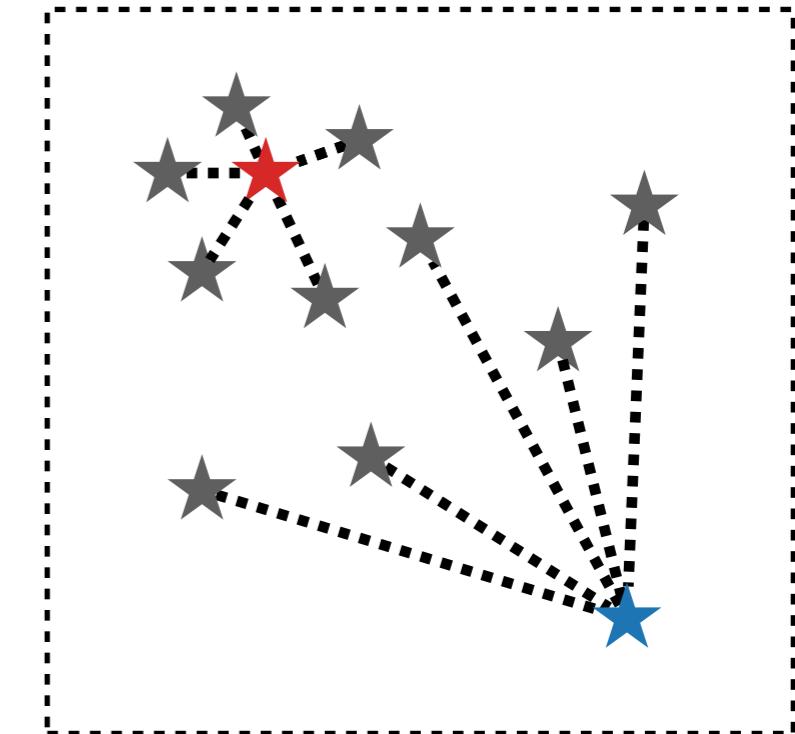
# Least Representative Jets



[<http://opendata.cern.ch/>]



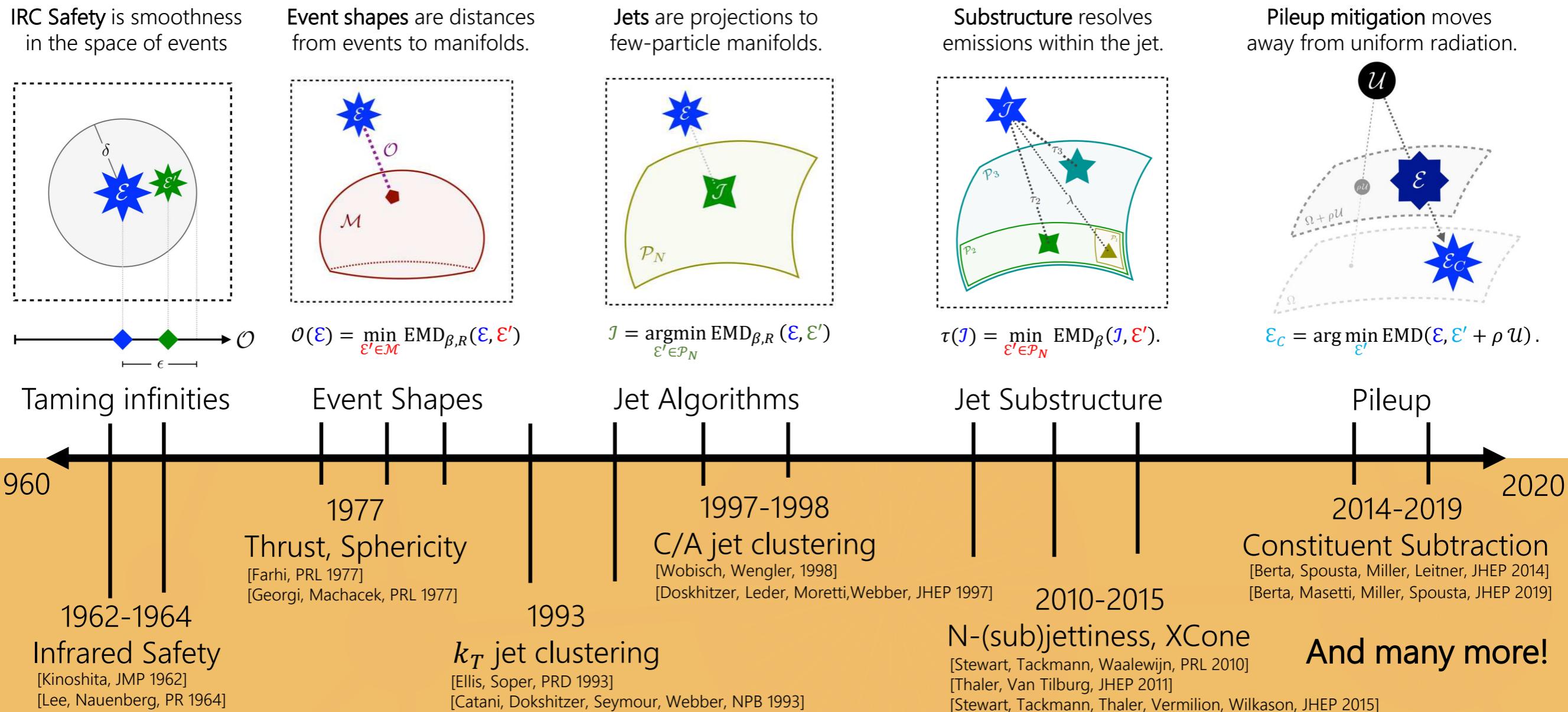
New Physics?  
Or tails of QCD?



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



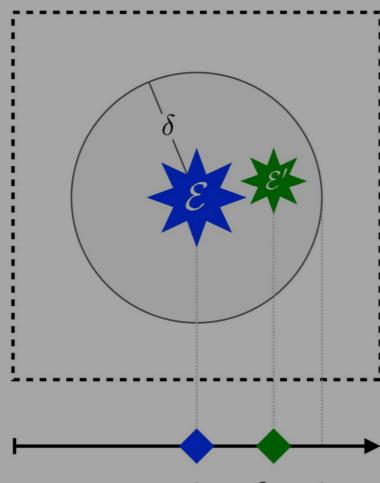
# Six Decades of Collider Physics Translated into a New Geometric Language!



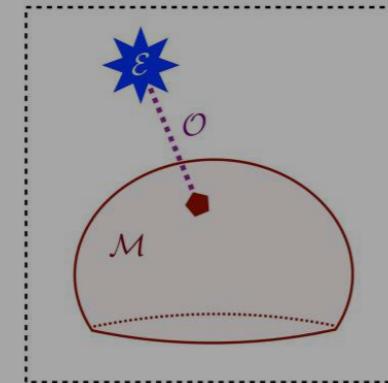
[Timeline from Eric Metodiev; Komiske, Metodiev, JDT, JHEP 2020]

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

IRC Safety is smoothness in the space of events



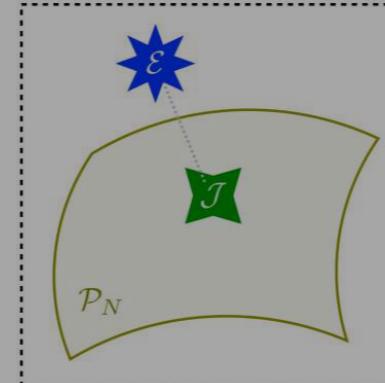
Event shapes are distances from events to manifolds.



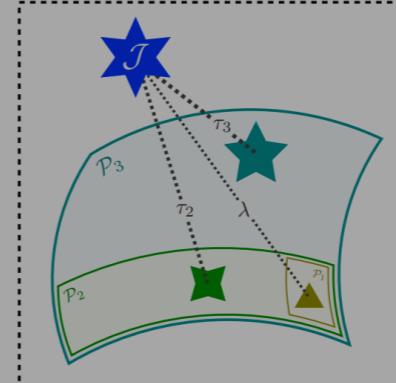
Taming infinities

Event Shapes

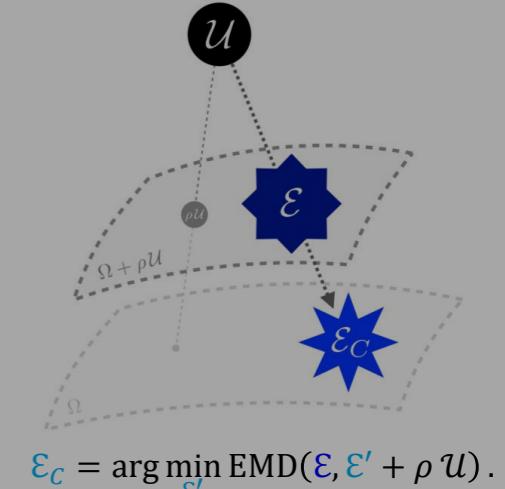
Jets are projections to few-particle manifolds.



Substructure resolves emissions within the jet.



Pileup mitigation moves away from uniform radiation.



1960

1962-1964

Infrared Safety  
[Kinoshita, JMP 1962]  
[Lee, Nauenberg, PR 1964]



1973

$k_T$  jet clustering  
[Ellis, Soper, PRD 1993]  
[Catani, Dokshitzer, Seymour, Webber, NPB 1993]

Jet Algorithms

1997-1998  
C/A jet clustering  
[Wobisch, Wengler, 1998]  
[Dokshitzer, Leder, Moretti, Webber, JHEP 1997]

Jet Substructure

2010-2015

N-(sub)jettiness, XCone  
[Stewart, Tackmann, Waalewijn, PRL 2010]  
[Thaler, Van Tilburg, JHEP 2011]  
[Stewart, Tackmann, Thaler, Vermilion, Wilkason, JHEP 2015]

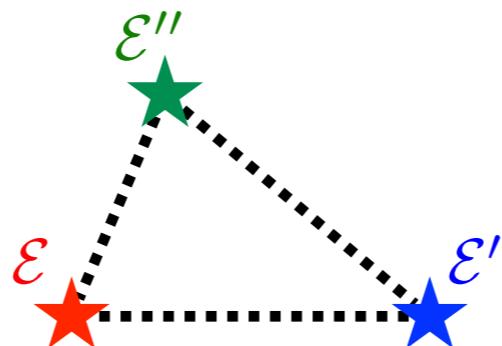
Pileup

2014-2019

Constituent Subtraction  
[Berta, Spousta, Miller, Leitner, JHEP 2014]  
[Berta, Masetti, Miller, Spousta, JHEP 2019]

And many more!

[Timeline from Eric Metodiev; Komiske, Metodiev, JDT, JHEP 2020]

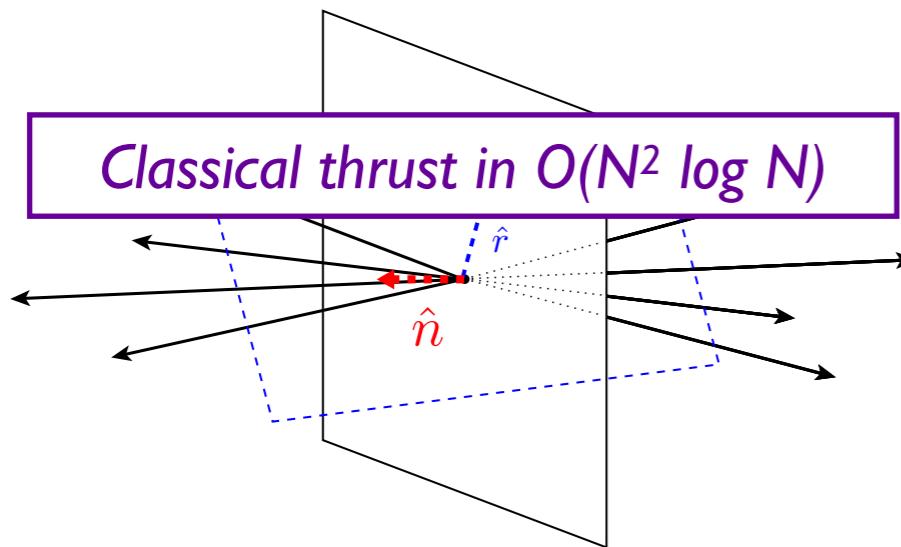


Quantum Inspiration:  
*Potential polynomial improvements over classical algorithms*

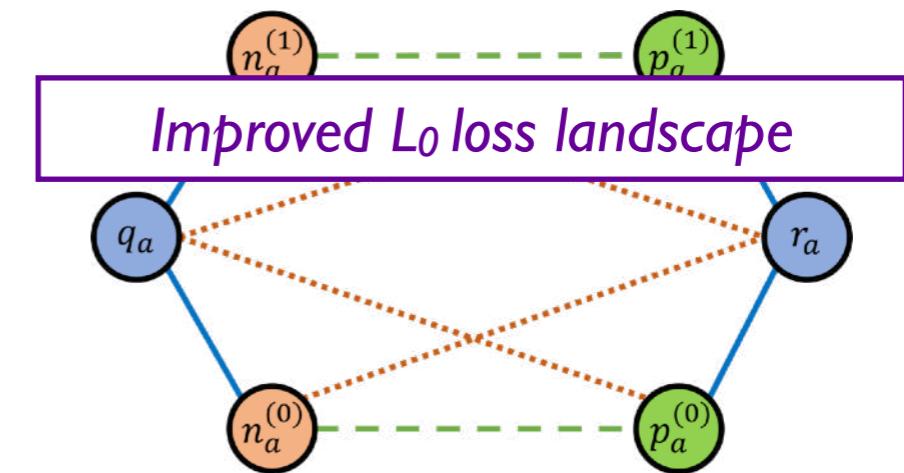
Classical Development:  
*New geometric data analysis strategy for collider physics*

# Quantum (Inspired) Algorithms for Colliders

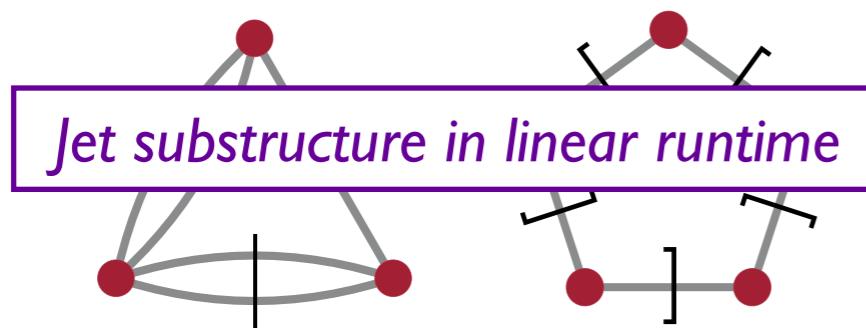
## Challenge of Data Loading



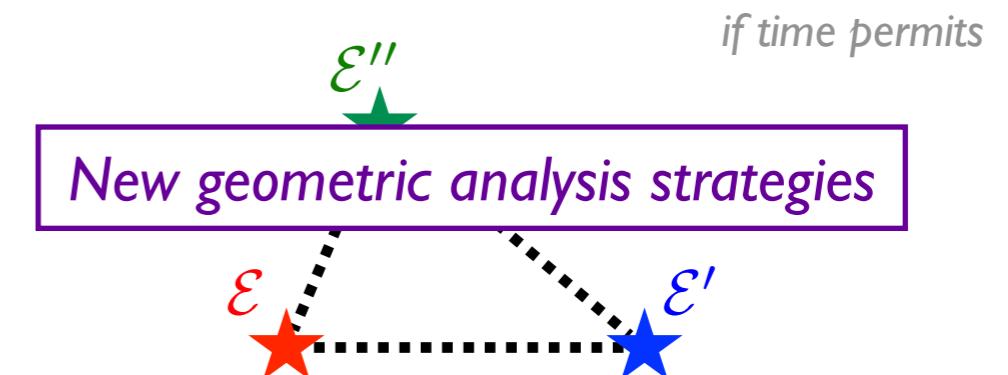
## Degeneracy Engineering



## Superposition for Graphs



## Optimal Transport



*Evangelizing one last time for QIS/HEP...*

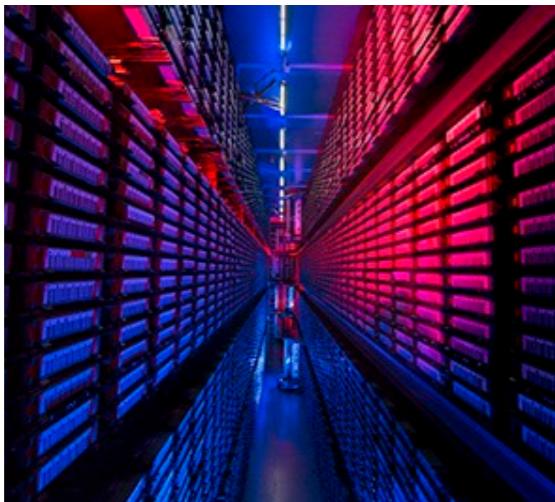
*Slides from 2020 pandemic slide deck*

# Quantum Algorithms for HEP

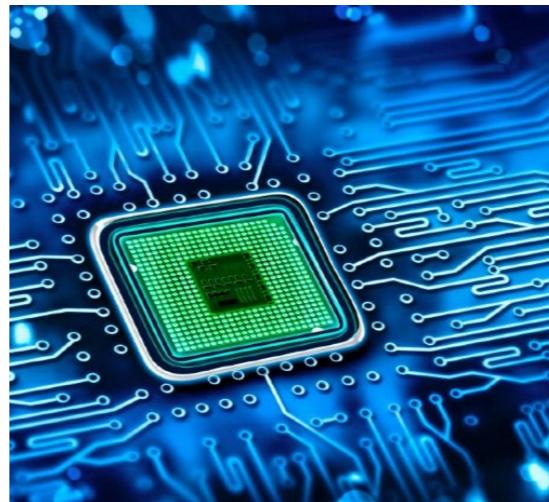
*Simulation, Reconstruction & Analysis*



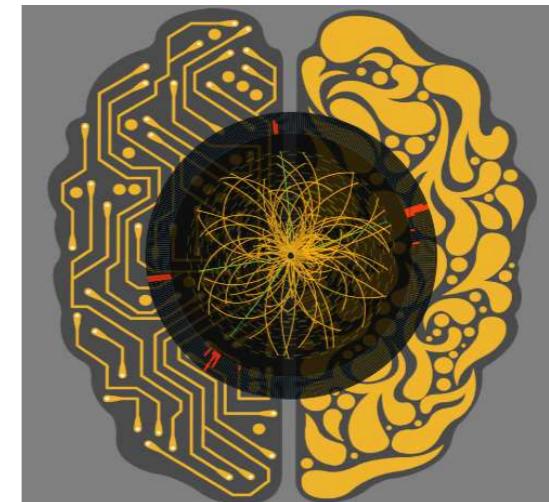
*High-energy physics has always been at the forefront of exploiting new computational technologies and algorithms*



Distributed Computing



Fast Inference



Machine Learning

...

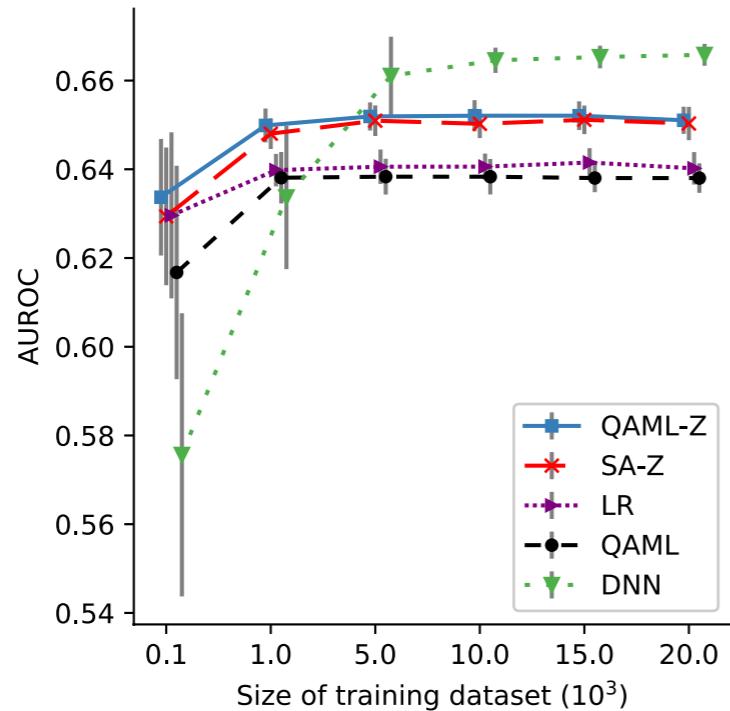
*Through new approaches to solve classically intractable problems,  
Quantum Computation could enable HEP discoveries*

*or at least inspire*

# *Backup Slides*

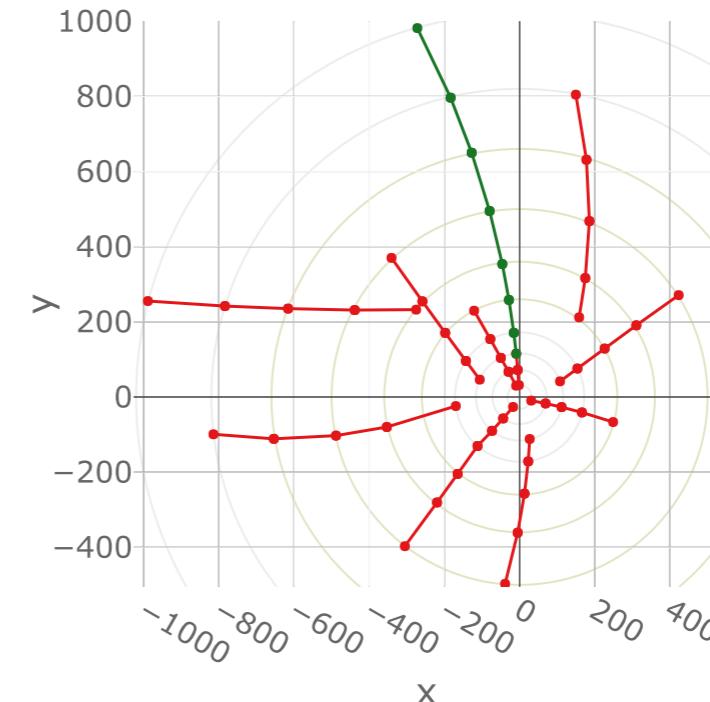
# Quantum Algorithms for HEP

## *Simulation, Reconstruction & Analysis*



### Higgs Boson Identification

[Mott, Job, Vlimant, Lidar, Spiropulu, [Nature 2017](#)]  
[Zlokapa, Mott, Job, Vlimant, Lidar, Spiropulu, [arXiv 2019](#)]



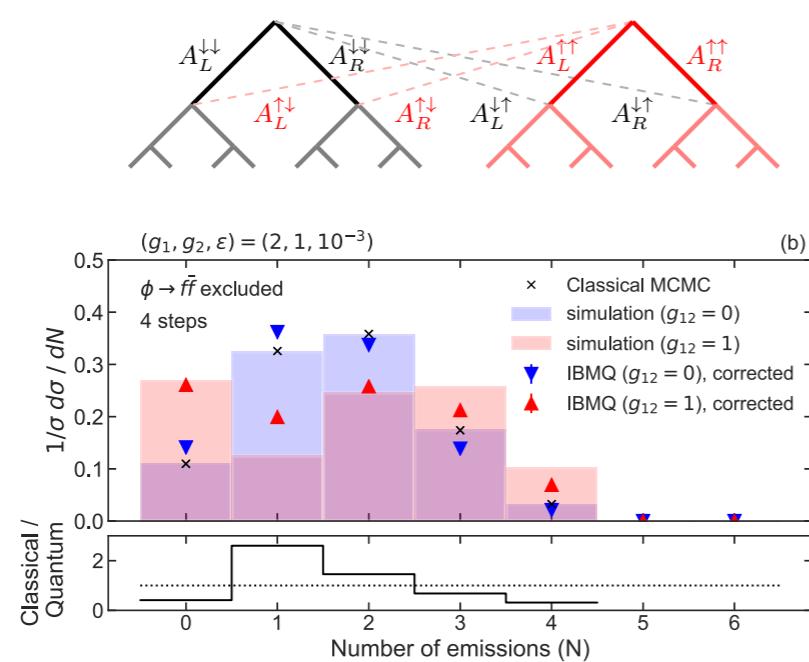
### Track Reconstruction

[Shapoval, Calafiura, [CHEP 2018](#)]  
[Bapst, Bhimji, Calafiura, Gray, Lavrijsen, Linder, [CSBS 2020](#)]  
[Zlokapa, Anand, Vlimant, Duarte, Job, Lidar, Spiropulu, [arXiv 2019](#)]

*Using quantum computation to confront the challenge of data interpretation at the LHC and other HEP experiments*

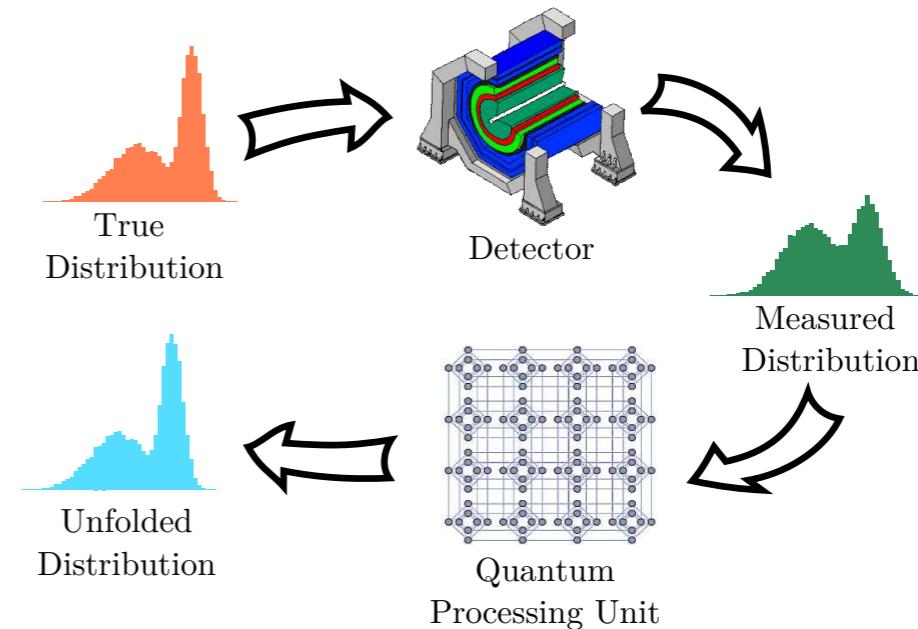
# Quantum Algorithms for HEP

## *Simulation, Reconstruction & Analysis*



### Parton Showers

[Provasoli, Nachman, de Jong, Bauer, [arXiv 2019](#)]  
 [Bauer, Nachman, Provasoli, de Jong, [arXiv 2019](#)]



### Detector Unfolding

[Cormier, Di Sipio, Wittek [JHEP 2019](#)]  
 [see also Nachman, Urbanek, de Jong, Bauer, [arXiv 2019](#)]

*Using quantum computation to confront the challenge of data interpretation at the LHC and other HEP experiments*

# Collider Event

Every 25 nanoseconds at the LHC

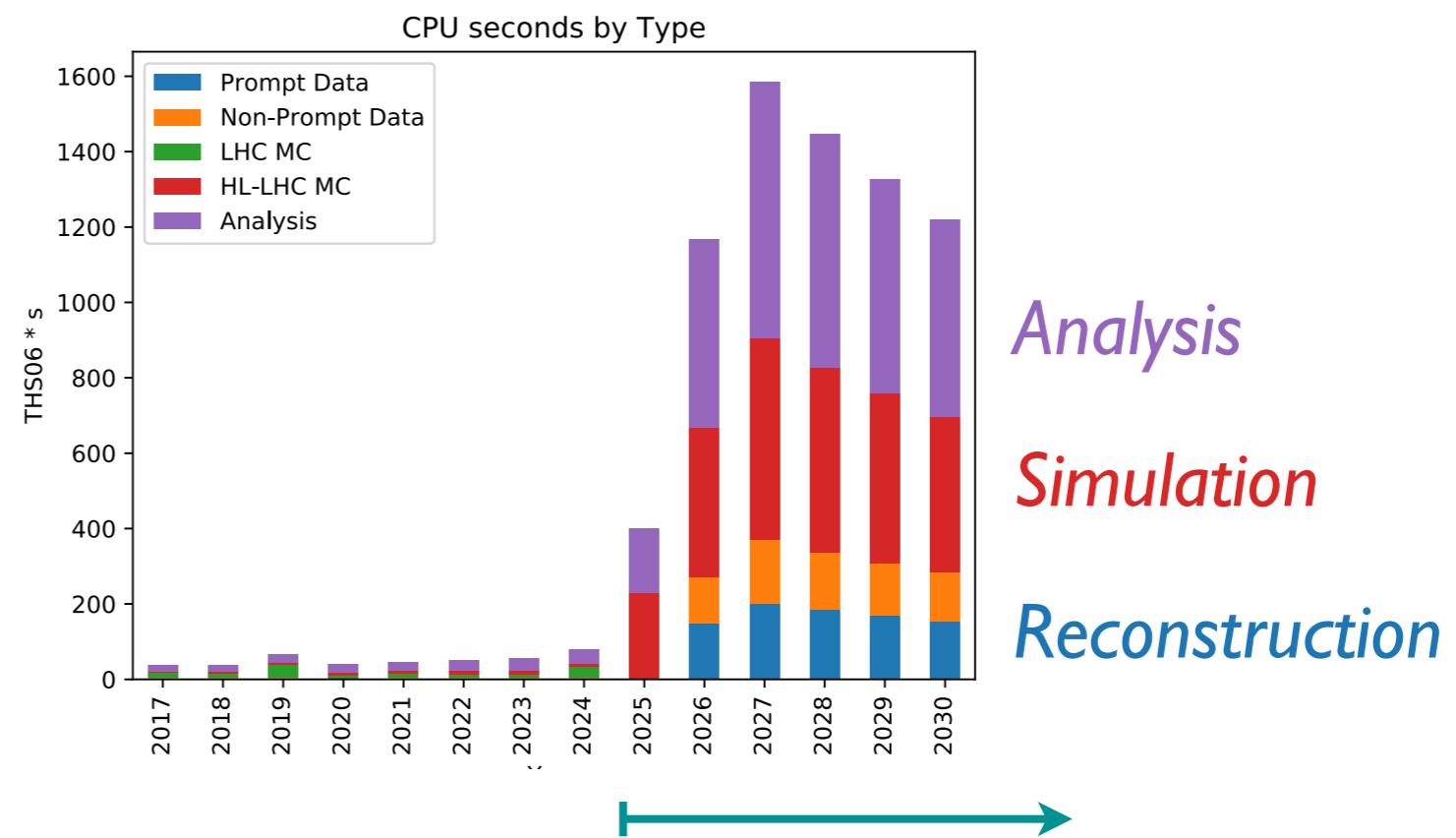
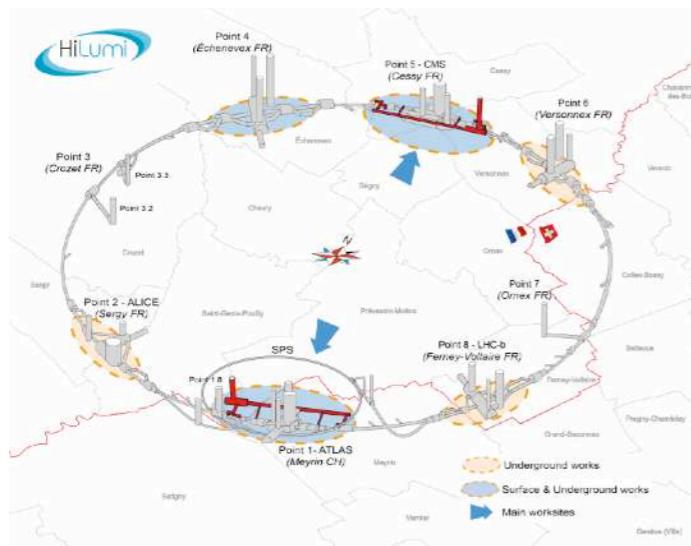
T E H M



$\gamma$  photon



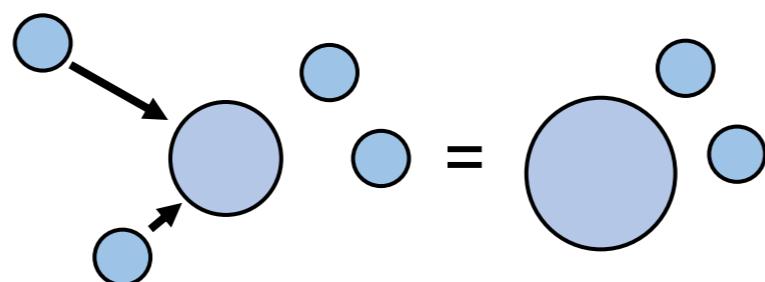
Ballooning computational costs for HL-LHC  
require near-term advances (presumably classical)



*Strong motivation for quantum research, but can it fight  $O(N)$ ?*

[HEP Software Foundation, [CSBS 2019](#), HSF Physics Event Generator Working Group, [CSBS 2021](#)]

## Connections to Chemistry

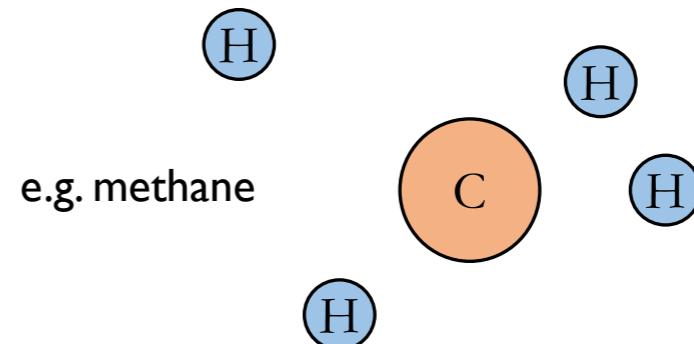


# Molecular Symmetries and Quantum Field Theory?

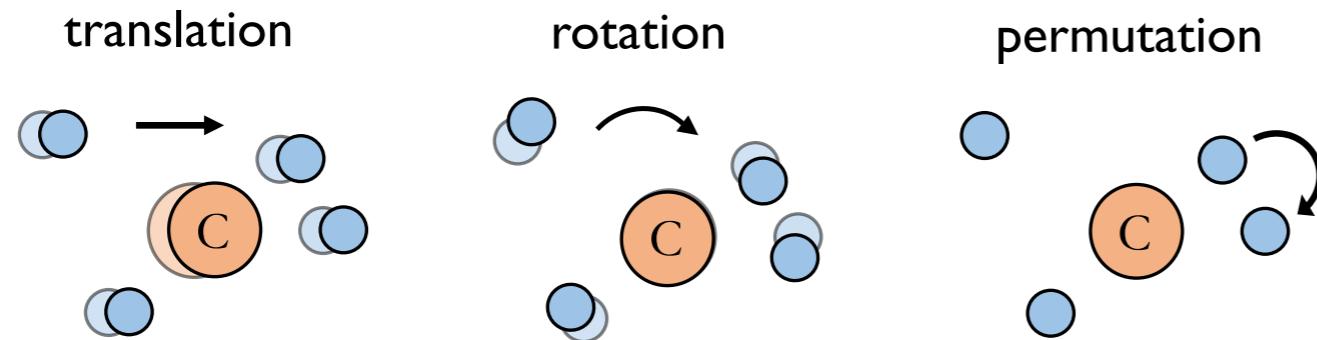
What is the ground state energy of a collection of atoms?

$$E(\{Z_i, \vec{r}_i\}_{i=1}^{n_N})$$

nuclear charges      nuclear positions



What are the symmetries of  $E$ ?



Are there hidden symmetries?

$$H = \underbrace{\frac{\hbar}{2m_e} \sum_{i \in e}^{n_e} \nabla_i^2}_{\text{electron kinetic terms}} + \underbrace{\frac{e^2}{4\pi\epsilon_0} \left[ \sum_{i \in e}^{n_e} \sum_{j < i} \frac{1}{|\vec{r}_i - \vec{r}_j|} - \sum_{i \in e}^{n_e} \sum_{j \in N} \frac{Z_j}{|\vec{r}_i - \vec{r}_j|} \right]}_{\text{electron-electron repulsion, electron-nucleus attraction}} + \underbrace{\frac{e^2}{4\pi\epsilon_0} \sum_{i \in N}^{n_N} \sum_{j < i} \frac{Z_i Z_j}{|\vec{r}_i - \vec{r}_j|}}_{\text{nucleus-nucleus repulsion}}$$

$H_{\text{elec}}$  **Focus on Electronic Energy**

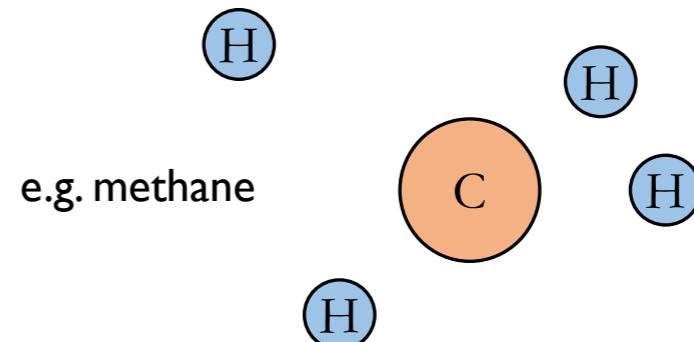
$V_{NN}$  **Known Analytically!**

# Molecular Symmetries and Quantum Field Theory?

What is the ground state **electronic** energy of a collection of atoms?

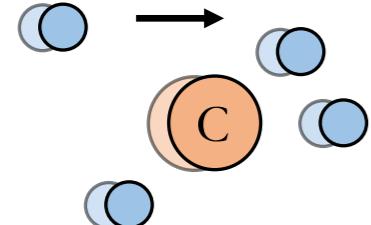
$$E_{\text{elec}}(\{Z_i, \vec{r}_i\}_{i=1}^{n_N})$$

nuclear charges      nuclear positions

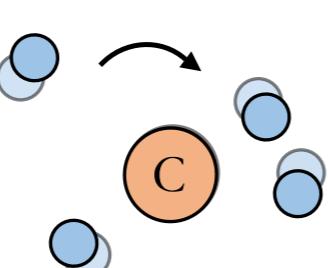


What are the symmetries of  $E_{\text{elec}}$ ?

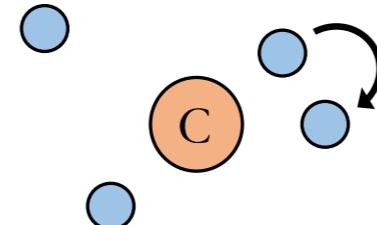
translation



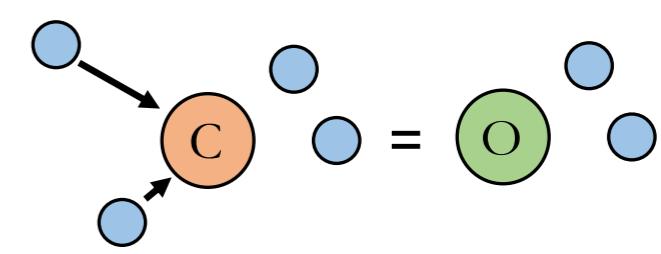
rotation



permutation

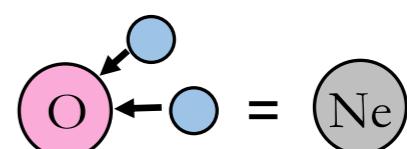
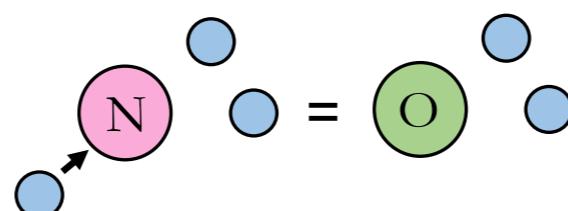
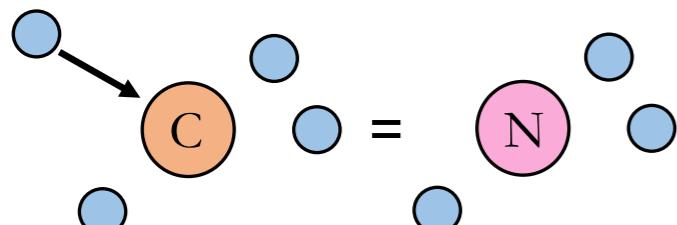


**united atom**



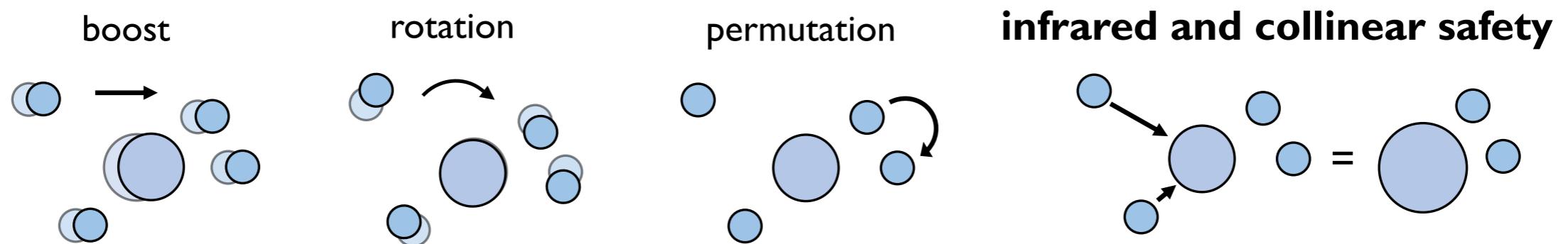
United Atom Symmetry is extremely constraining!

E.g.: knowing configuration energies of **methane** specifies properties of **ammonia** and **water**.



# Molecular Symmetries and Quantum Field Theory?

What are the symmetries of (perturbatively-calculable) scattering observables?



Mathematically identical to the molecular symmetries!



**Ongoing work:** We can directly apply our developments from collider physics.

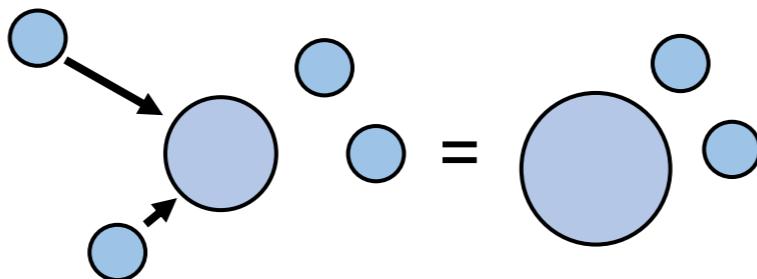
Fit to all molecules simultaneously! Also solves problems with “holes” in the fits.

Polynomial basis with full symmetries  
[\[Komiske, Metodiev, Thaler 1712.07124\]](#)

$$\sum_{i_1 \in N}^{n_N} \sum_{i_2 \in N}^{n_N} \dots \sum_{i_M \in N}^{n_N} Z_{i_1} Z_{i_2} \dots Z_{i_M} \prod_{(k,\ell) \in G} \theta_{i_k i_\ell}$$

Symmetric machine learning architecture for molecules

[\[Komiske, Metodiev, Thaler 1810.05165\]](#)

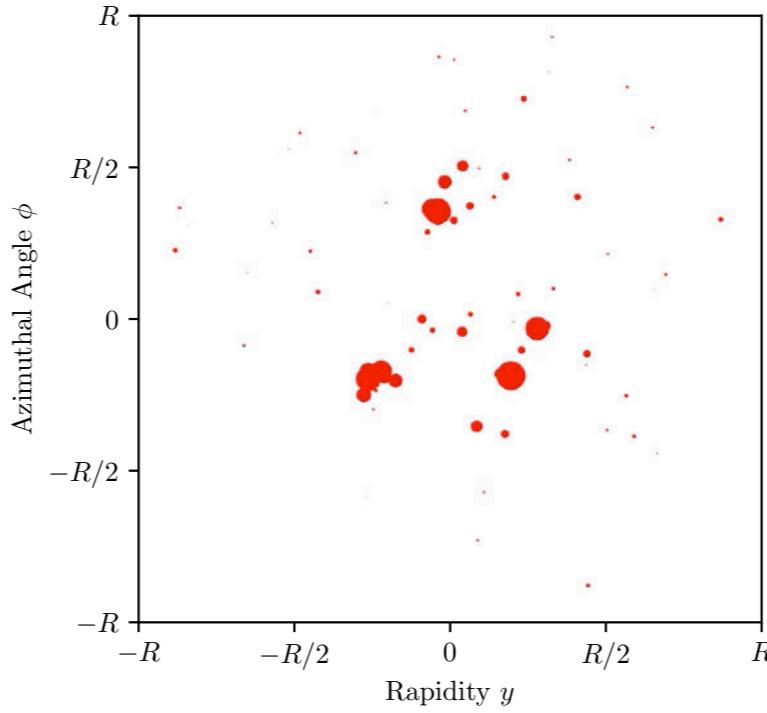


**Quantum Inspiration:**  
*Encoding symmetries of electron wave functions*

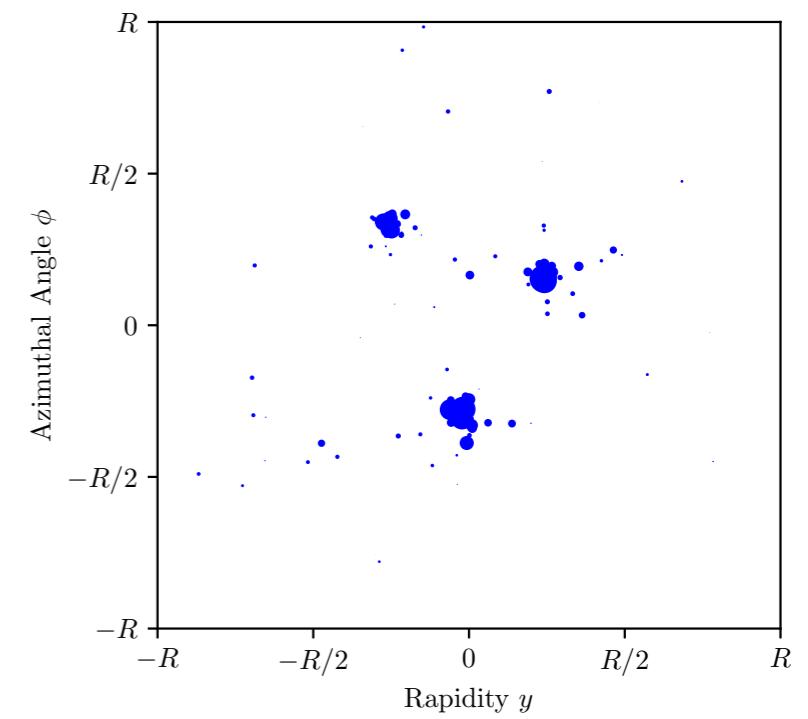
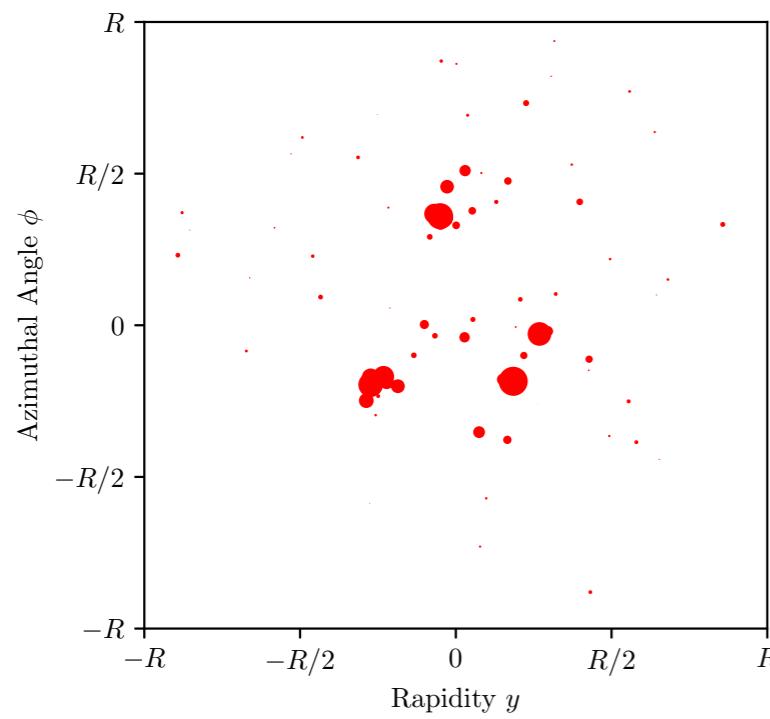
**Classical Development:**  
*Map between IRC safety (QFT) and united atom (chemistry)*

# 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](#)]

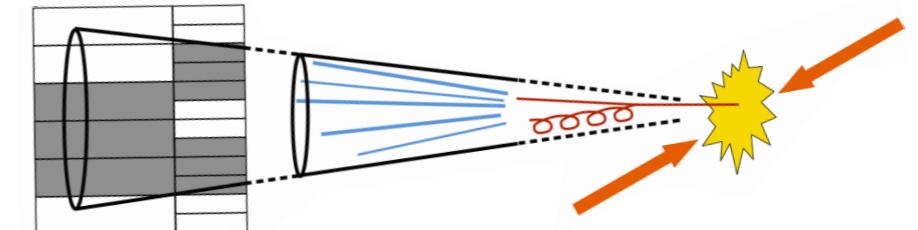
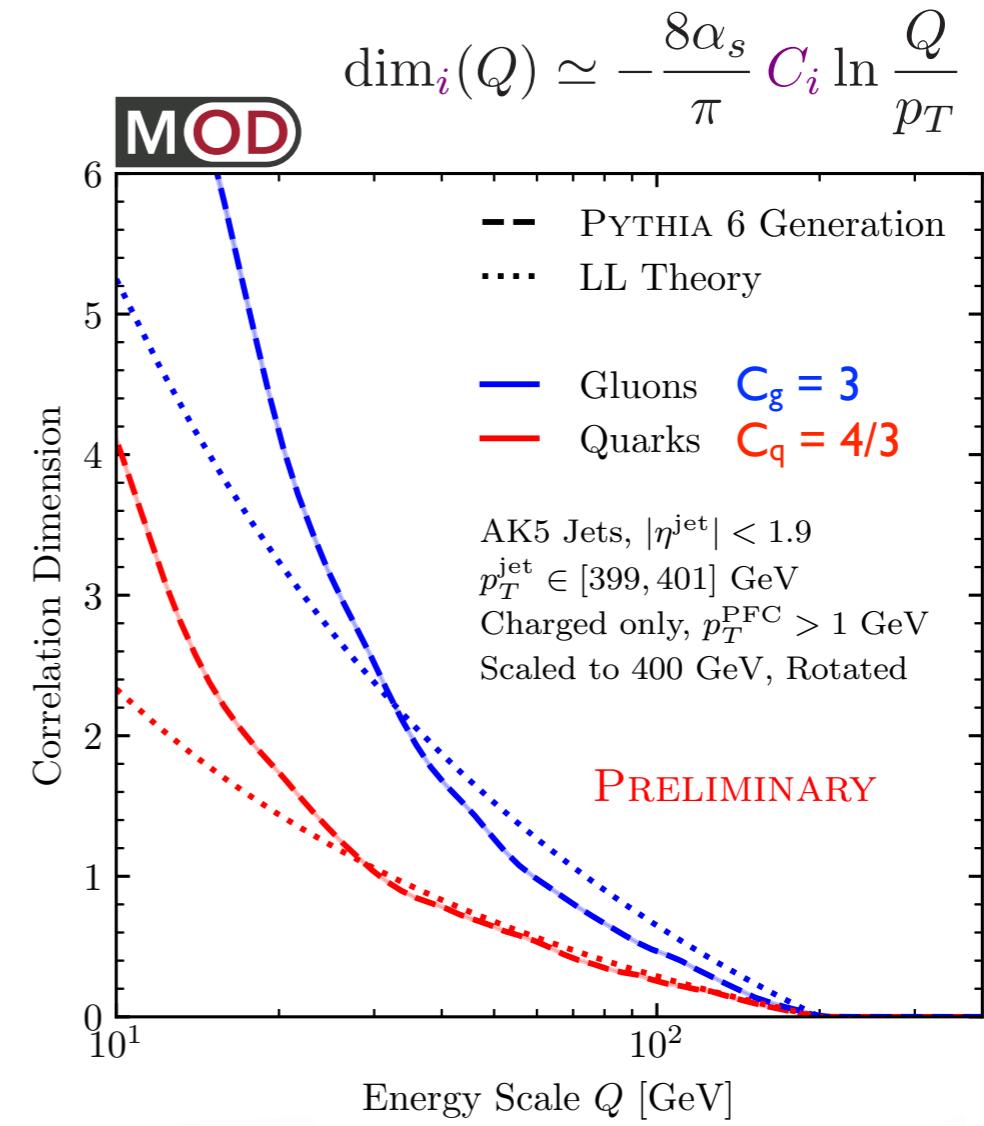
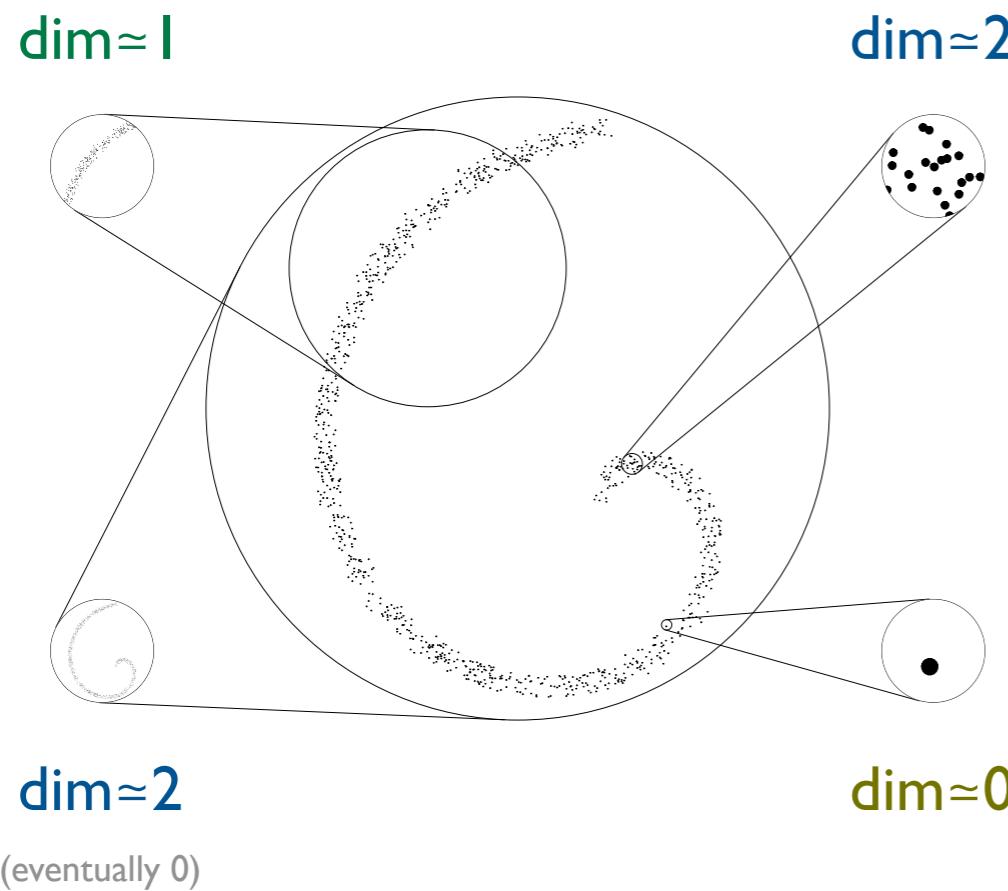
# Dimensionality of Space of Jets



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

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

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



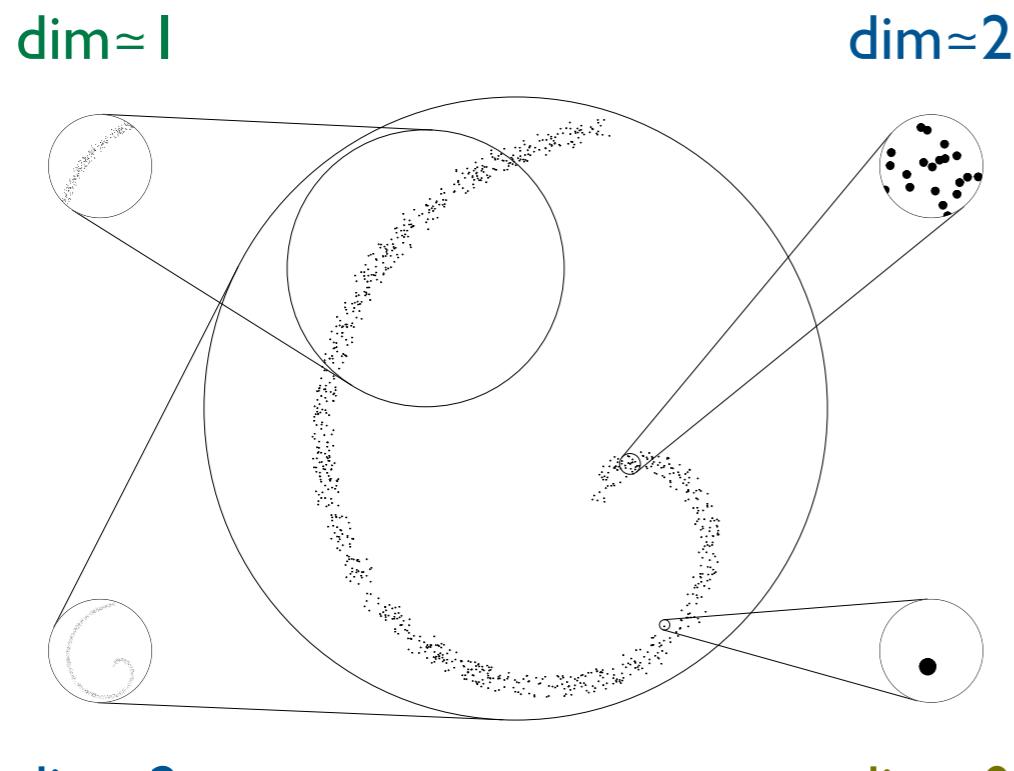
# Dimensionality of Space of Jets



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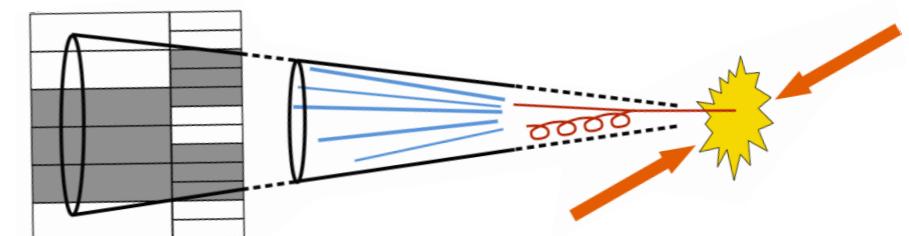
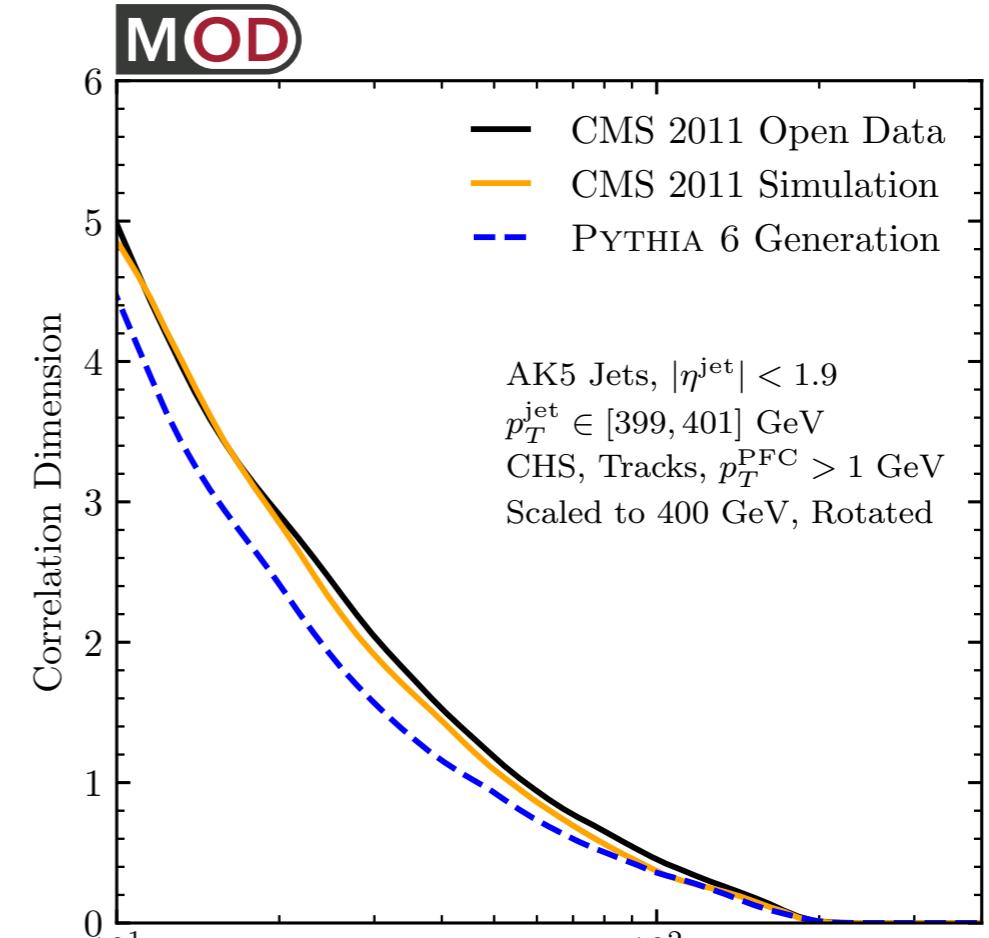
$$\Rightarrow \dim(r) \sim r \frac{\partial}{\partial r} \ln N_{\text{neighbors}}(r)$$

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



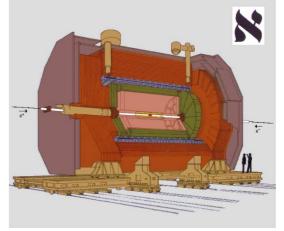
(eventually 0)

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

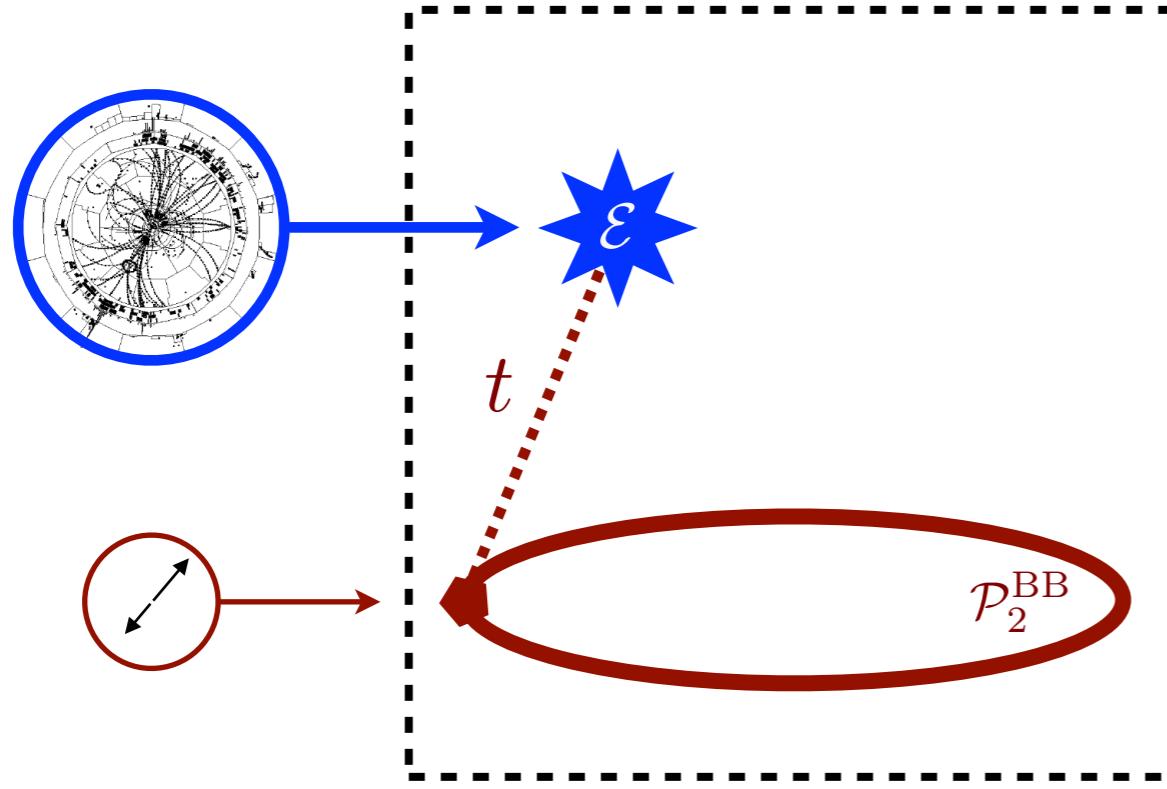


# E.g. Thrust

How dijet-like is an event?



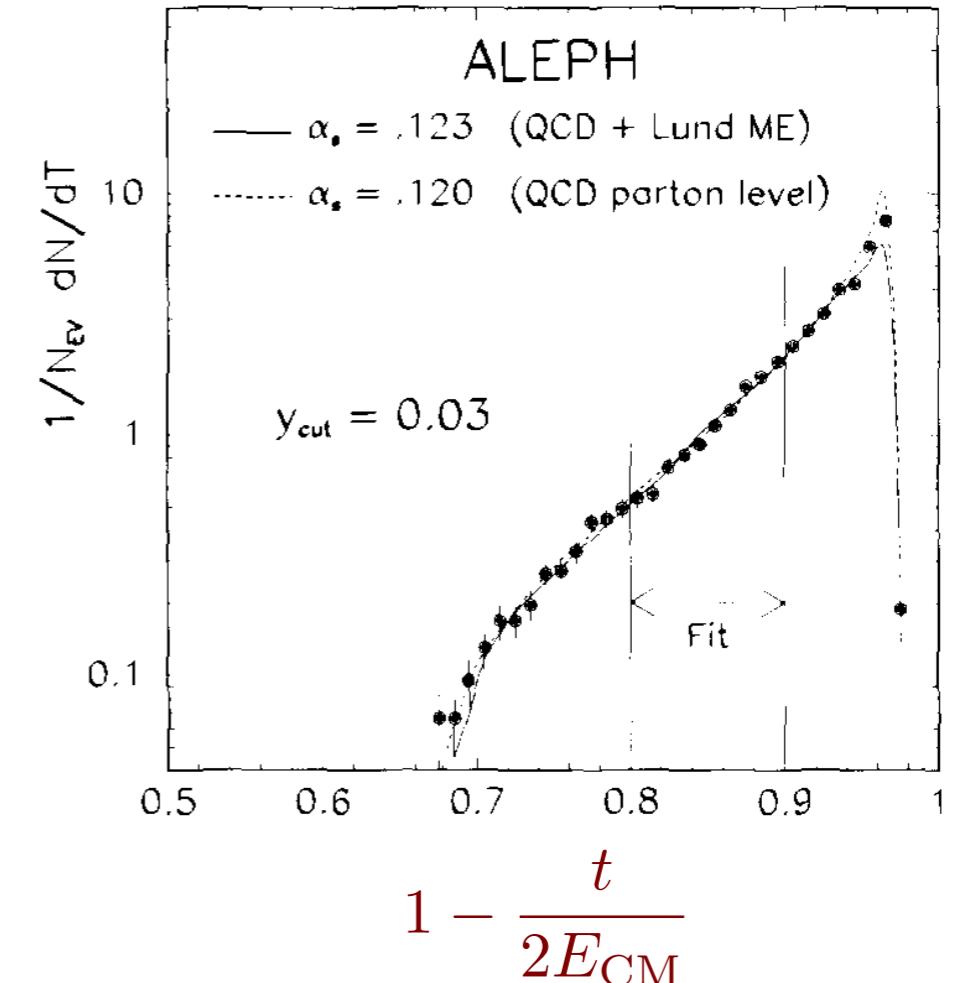
$$t(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{P}_2^{\text{BB}}} \text{EMD}_2(\mathcal{E}, \mathcal{E}')$$



All Back-to-Back Two Particle Configurations

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

(using  $\beta=2$  EMD variant)



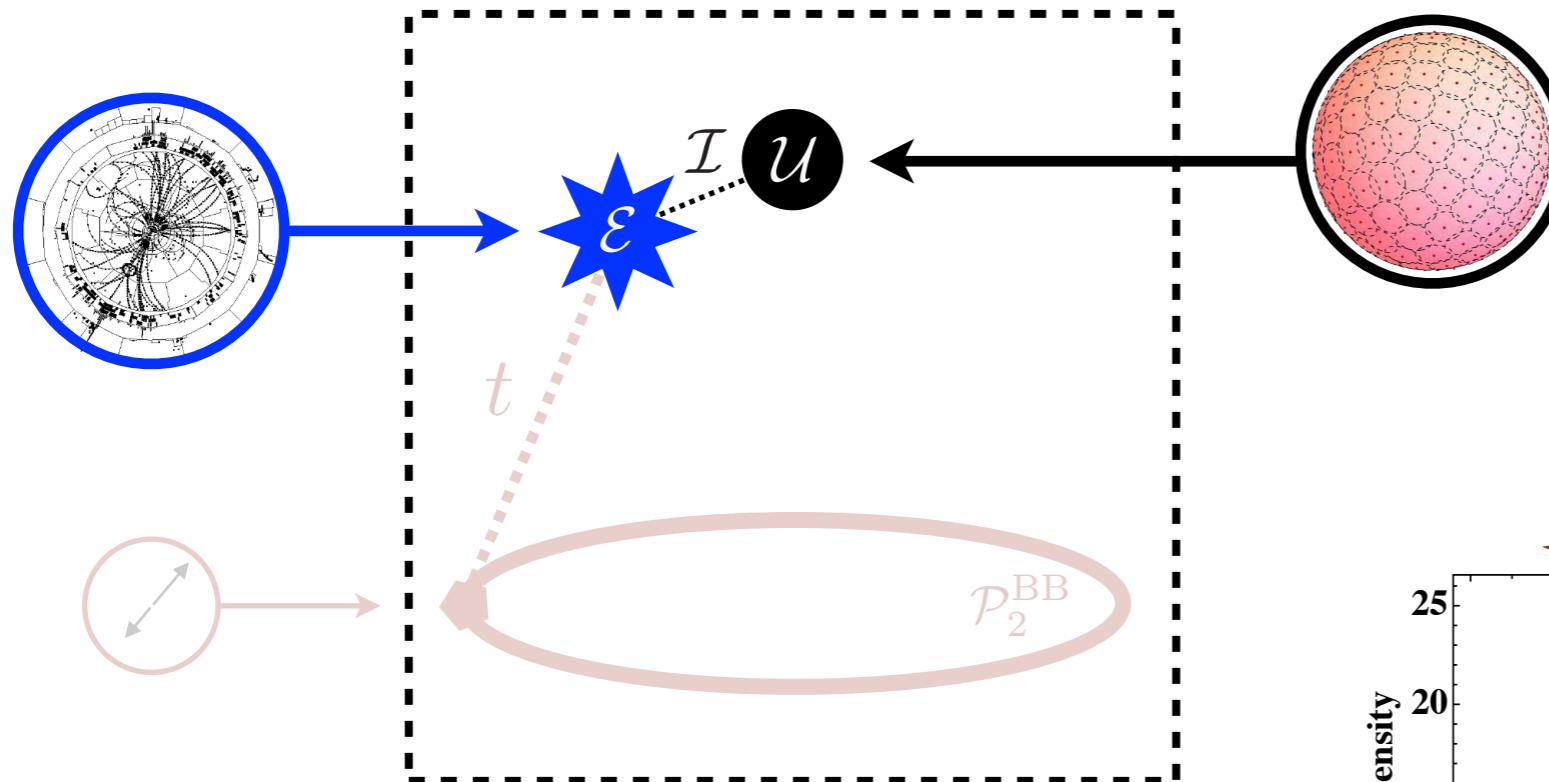
$$1 - \frac{t}{2E_{\text{CM}}}$$

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

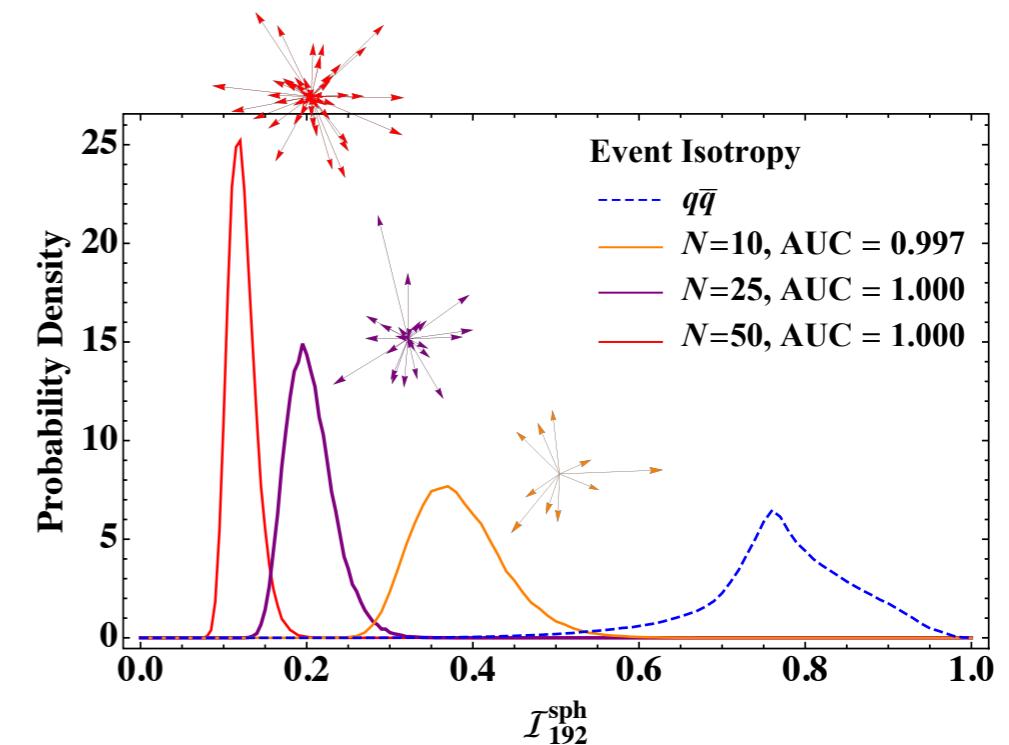
[Komiske, Metodiev, JDT, JHEP 2020]  
 [Brandt, Peyrou, Sosnowski, Wroblewski, PL 1964; Farhi, PRL 1977; ALEPH, PLB 1991]

# New! Event Isotropy

How isotropic is an event?



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



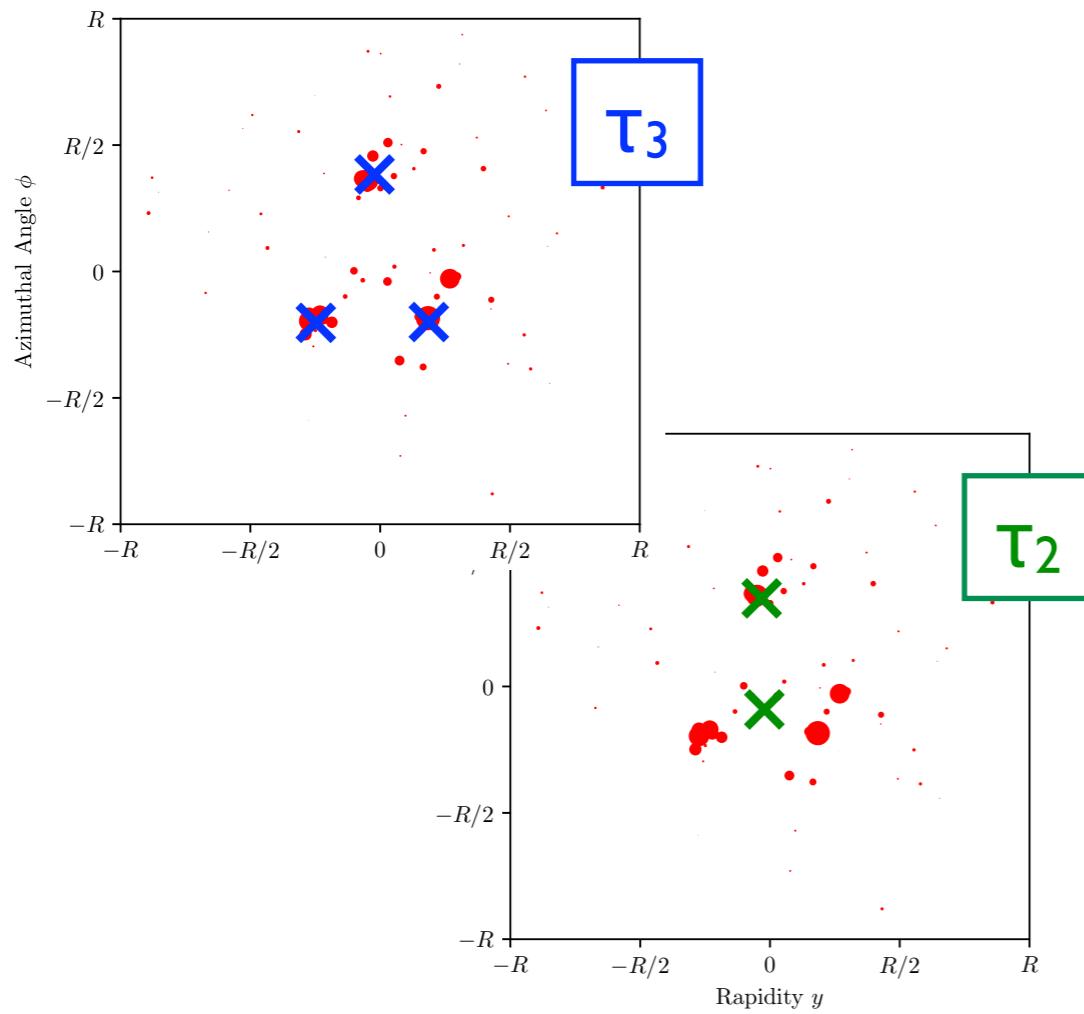
[Cesarotti, JDT, [JHEP 2020](#);  
see also Cesarotti, Reece, Strassler, [JHEP 2021](#)]



# N-subjettiness

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

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



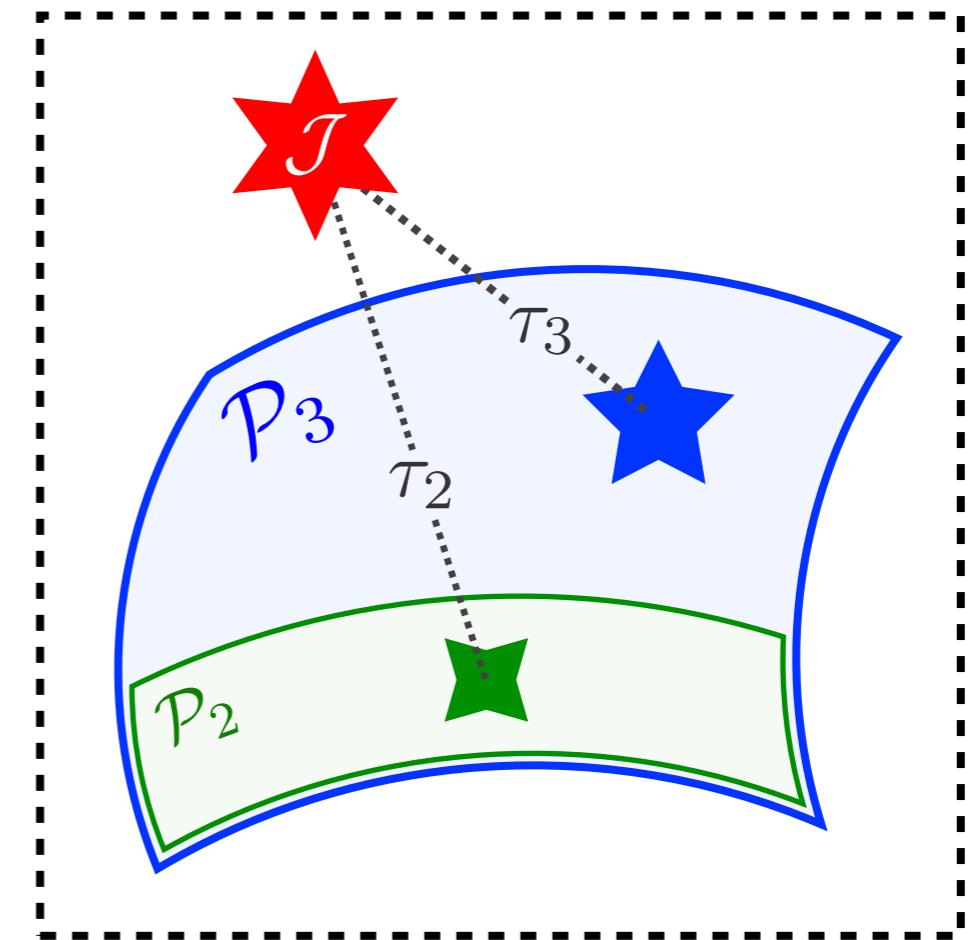
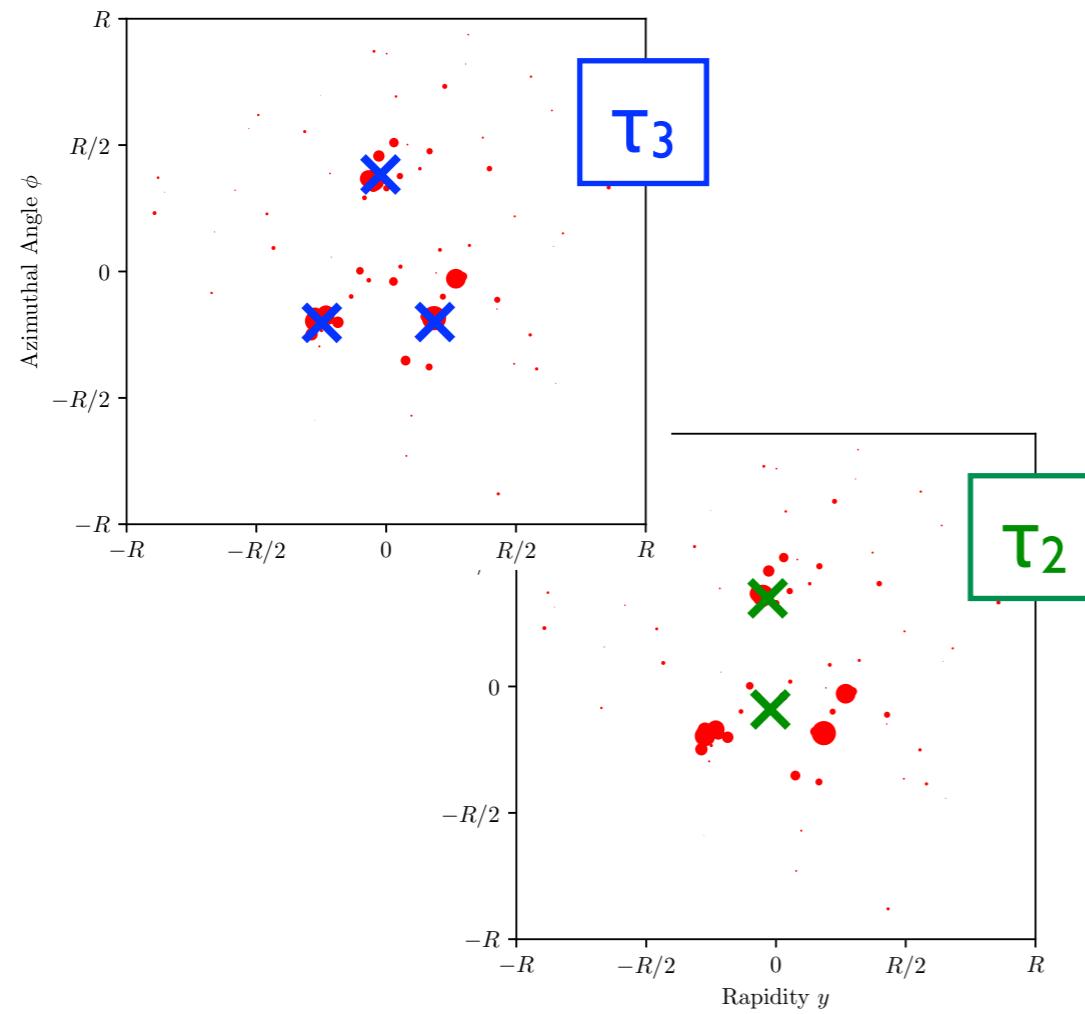
[JDT, Van Tilburg, [JHEP 2011](#), [JHEP 2012](#);  
based on Brandt, Dahmen, [ZPC 1979](#); Stewart, Tackmann, Waalewijn, [PRL 2010](#)]



# N-subjettiness = Point to Manifold EMD

*...is secretly an optimal transport problem*

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

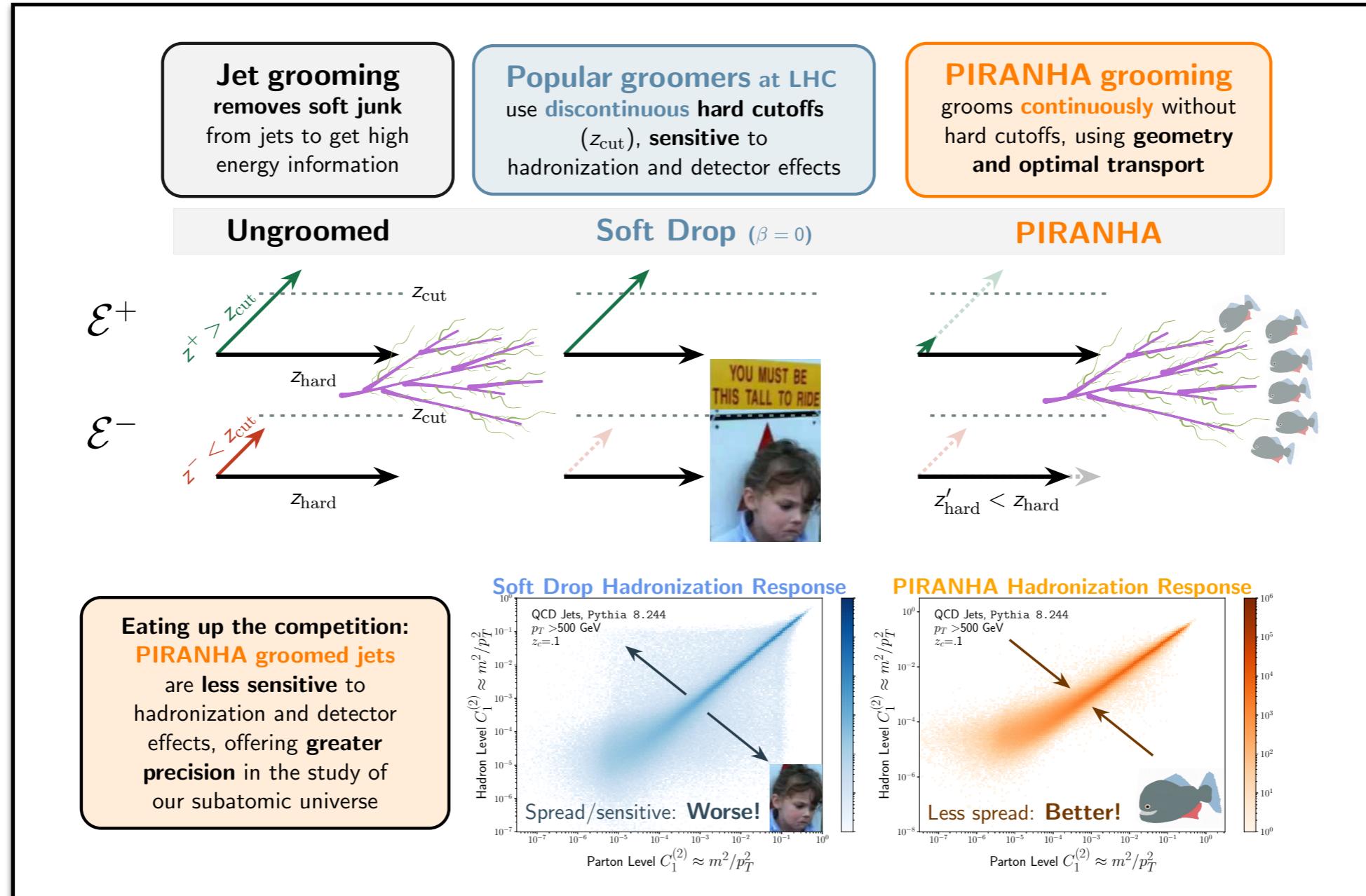


[JDT, Van Tilburg, JHEP 2011, JHEP 2012;  
rephrased in the language of Komiske, Metodiev, JDT, PRL 2019]



# 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]

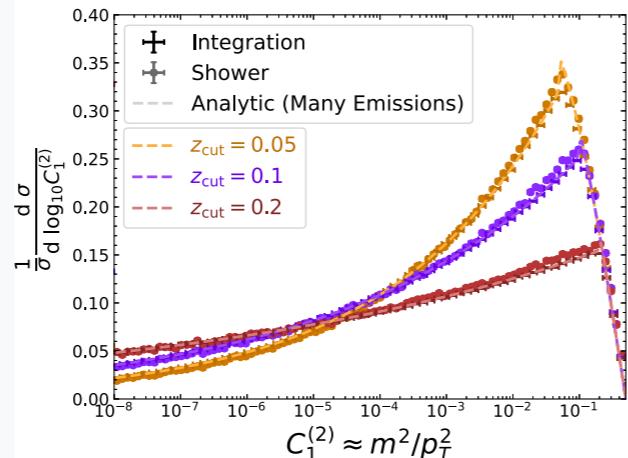


# Pileup and Infrared Radiation AnNiHilAtion

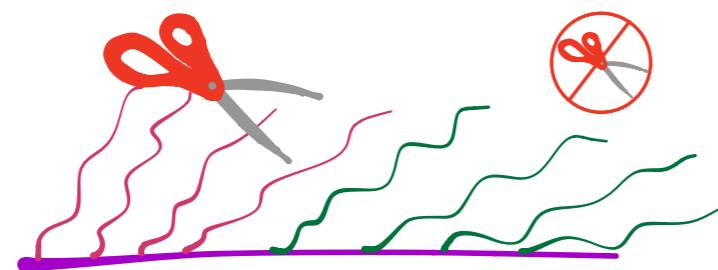
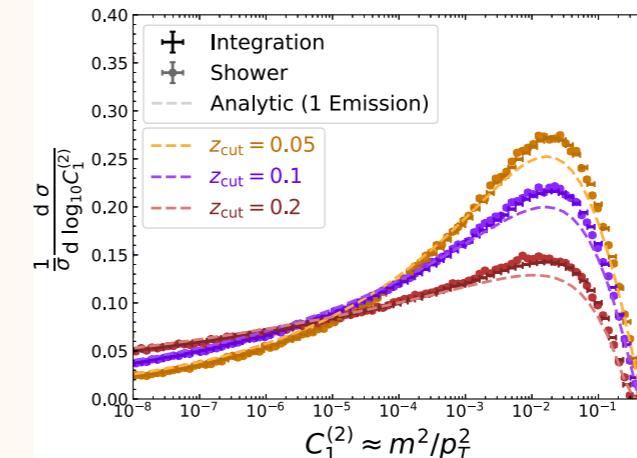
Recursive Safe Subtraction: tree-based approx. to optimal transport grooming

Fixed coupling, **multiple emission** calculations:

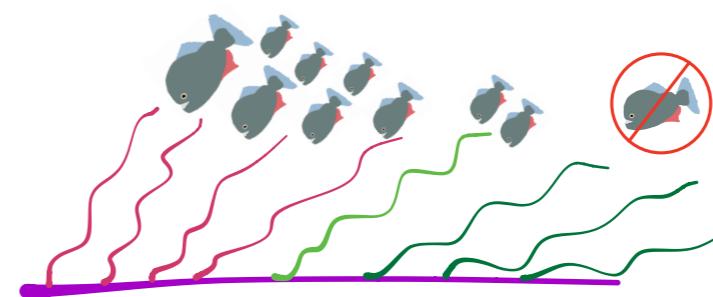
## Soft Drop/mMDT



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



Sharp cutoff → kink



No sharp cutoff → smooth

[Slides from Sam Alipour-fard]

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

