Quantum (Inspired) Algorithms for Collider Physics

Jesse Thaler

MIT

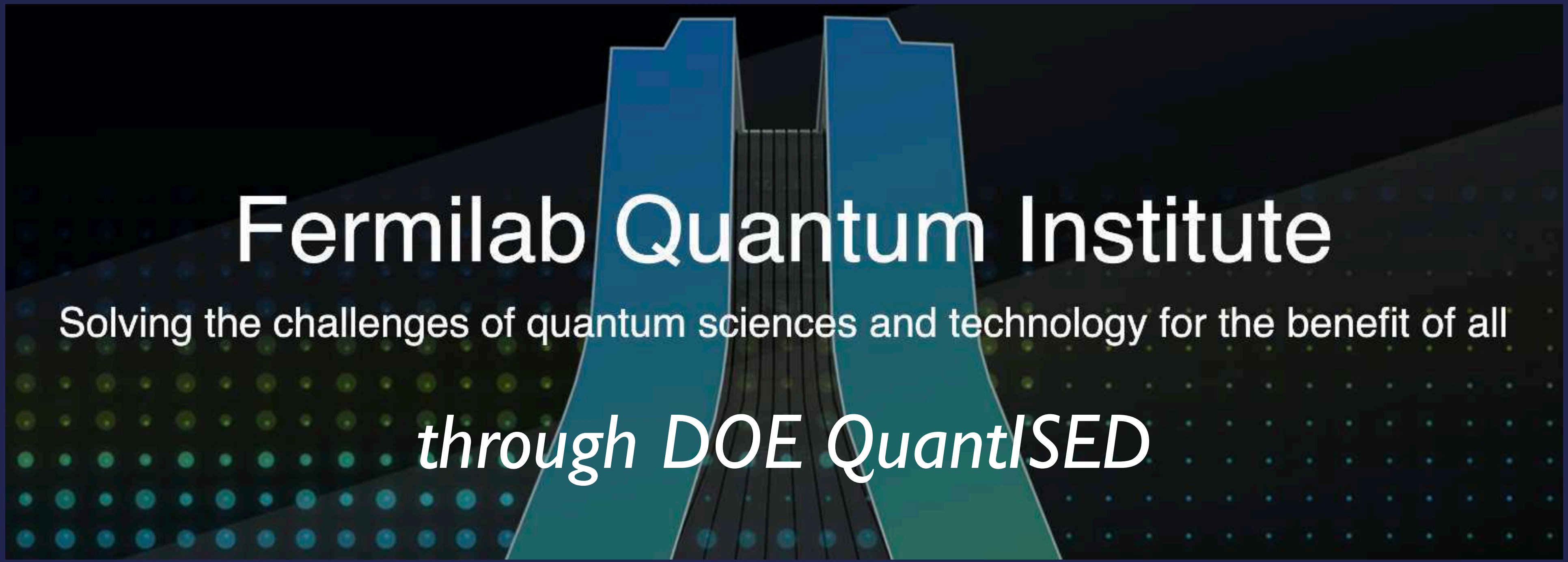
EPP Theory Seminar, SLAC — April 13, 2022

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]

C^{2}QA
Co-design Center for
Quantum Advantage



through DOE QuantISED

Why "Inspired"?

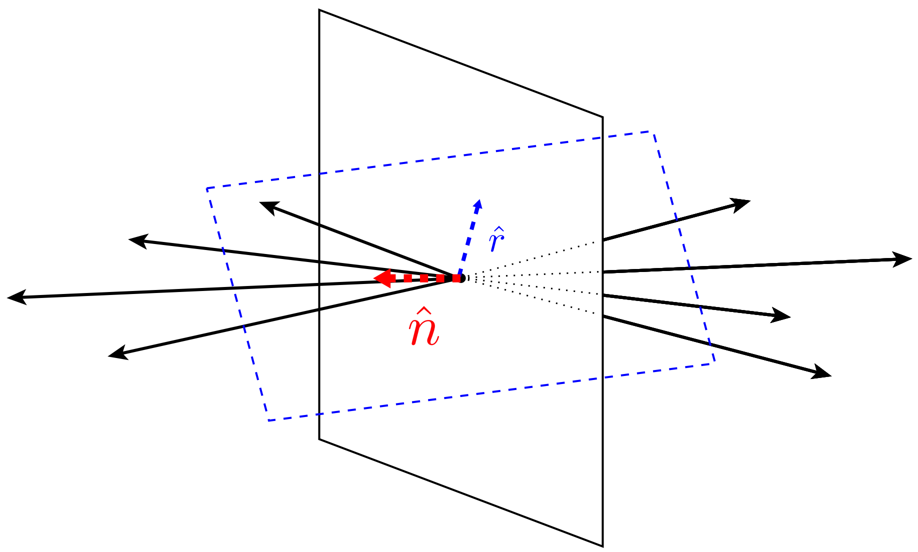
For the foreseeable future, data collected from colliders like the LHC will be classical

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

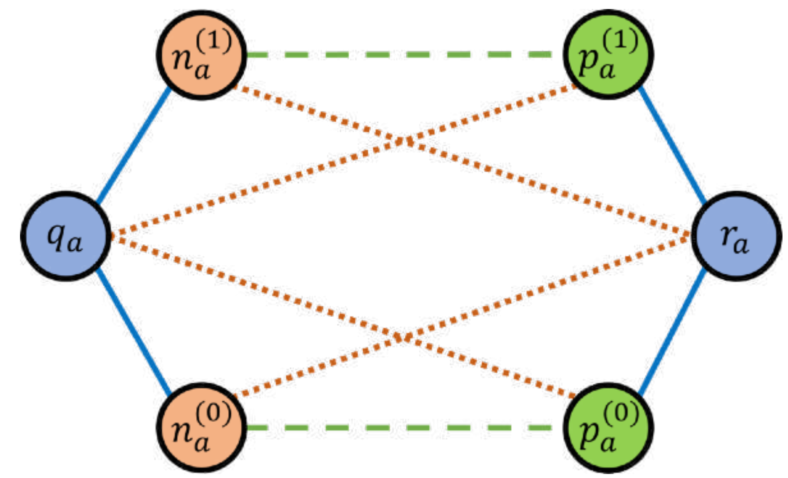
But quantum principles (e.g. superposition) and quantum challenges (e.g. data loading) have already inspired new classical algorithms

Four Quantum (Inspired) Anecdotes

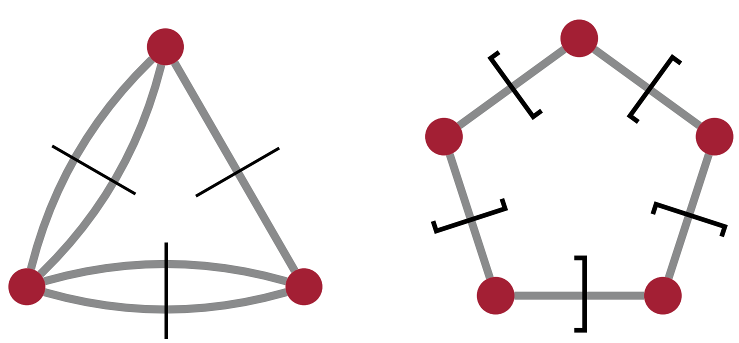
Challenge of Data Loading



Degeneracy Engineering

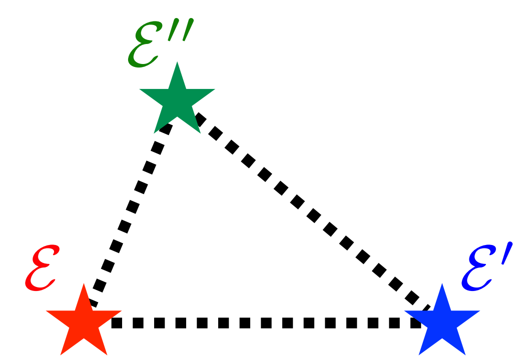


Superposition for Graphs



Optimal Transport

if time permits



First, evangelizing for QIS/HEP…

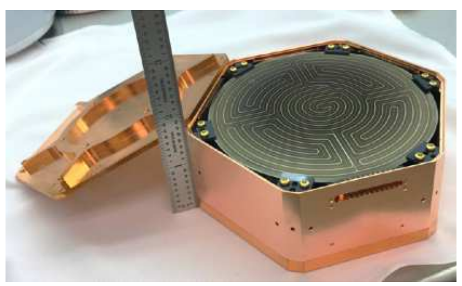
Slides from 2019 HEPAP presentation

HEP and the National Quantum Initiative

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

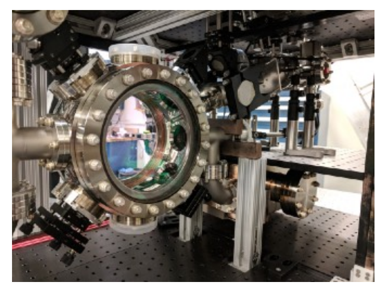
Already developing/exploiting Quantum Sensing technologies

Transition Edge Sensors



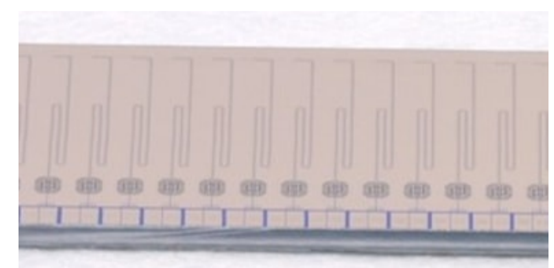
[SuperCDMS]

Atom Interferometry



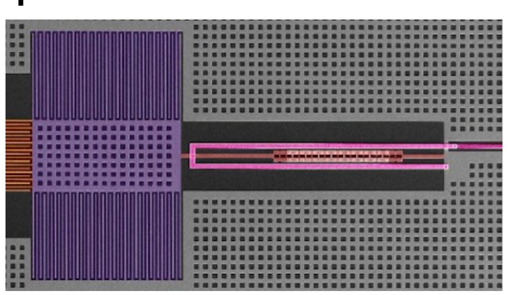
[MAGIS-100]

Microwave SQUID Multiplexers



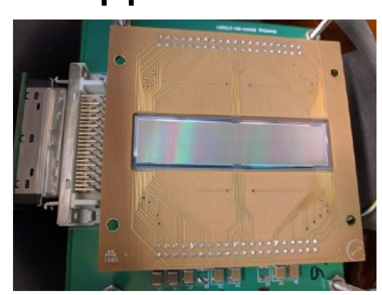
[Simons Observatory]

Squeezed State Receivers



[HAYSTAC]

Skipper CCDs



[SENSEI]

And More!

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

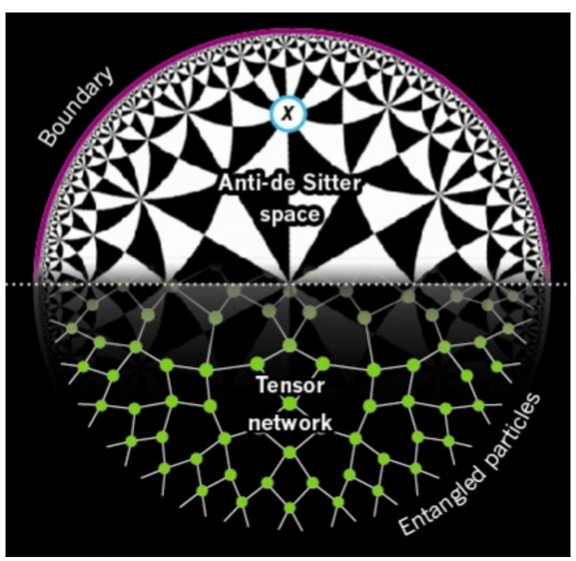
[see Nov 2018 HEPAP Meeting; Quantum Sensing for HEP (2018); 2019 Kavli ACP Workshop, Intersections QIS/HEP]

HEP and the National Quantum Initiative

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

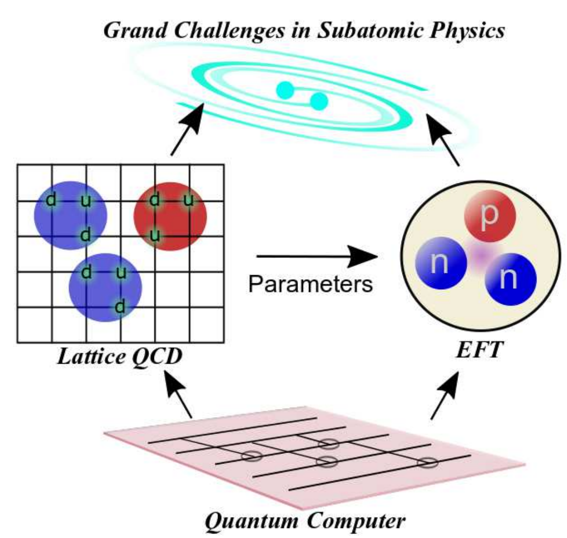
Fertile intersection between HEP and QIS
Potentially transformative, requires robust theory/R&D effort

Entanglement ⇔ Geometry



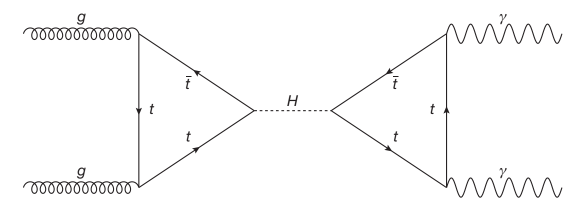
[figure from Nature 2015]

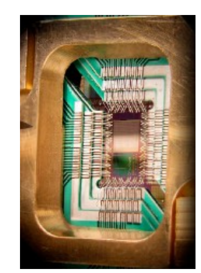
Simulation

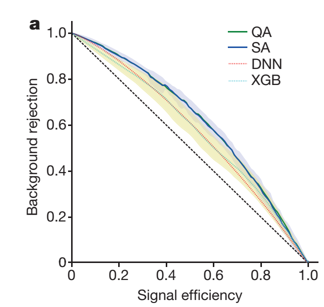


[figure from 1810.03959]

Computation/Analysis







[MJVLS, Nature 2017]

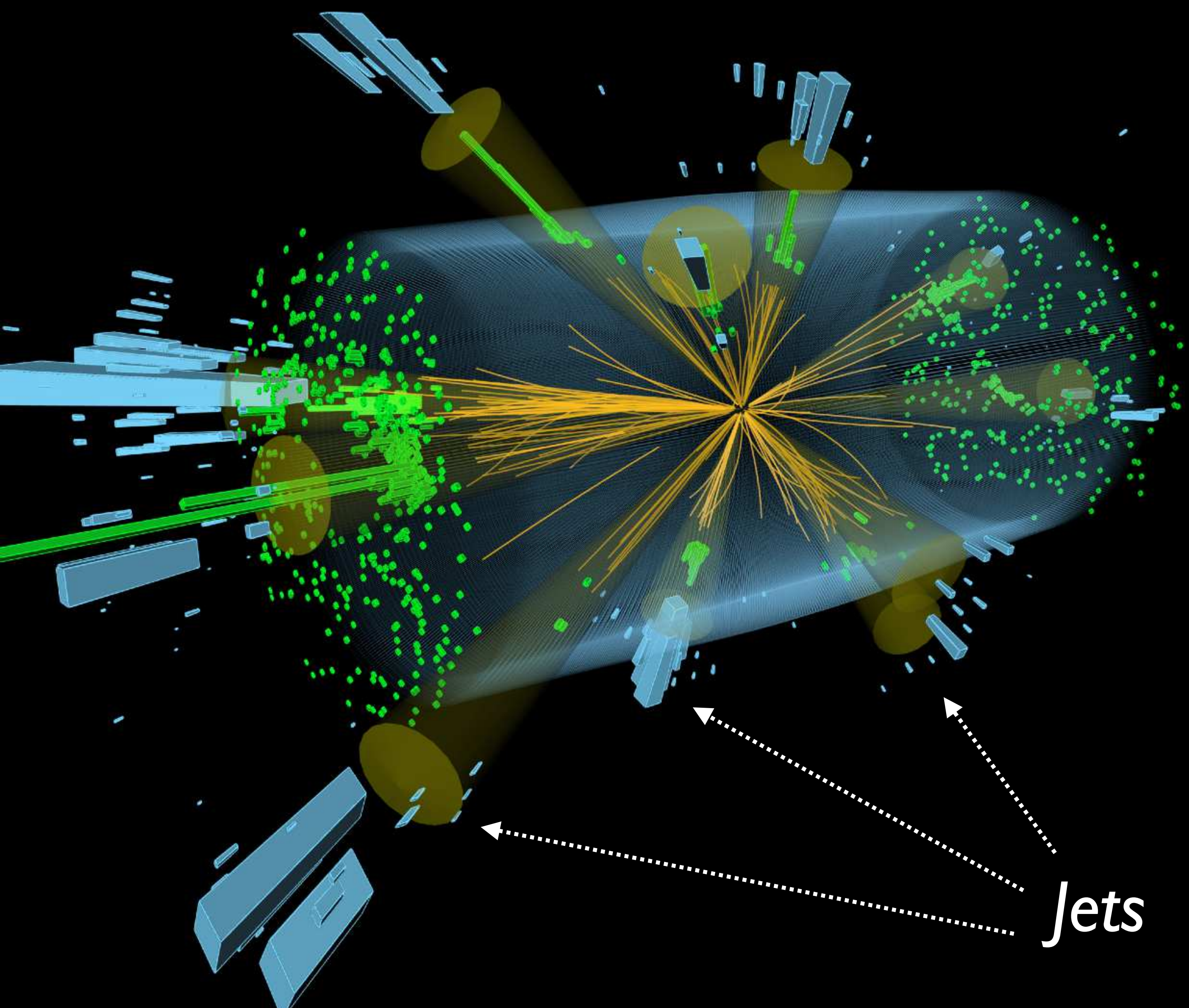
More evangelizing in backup

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

Collider Event

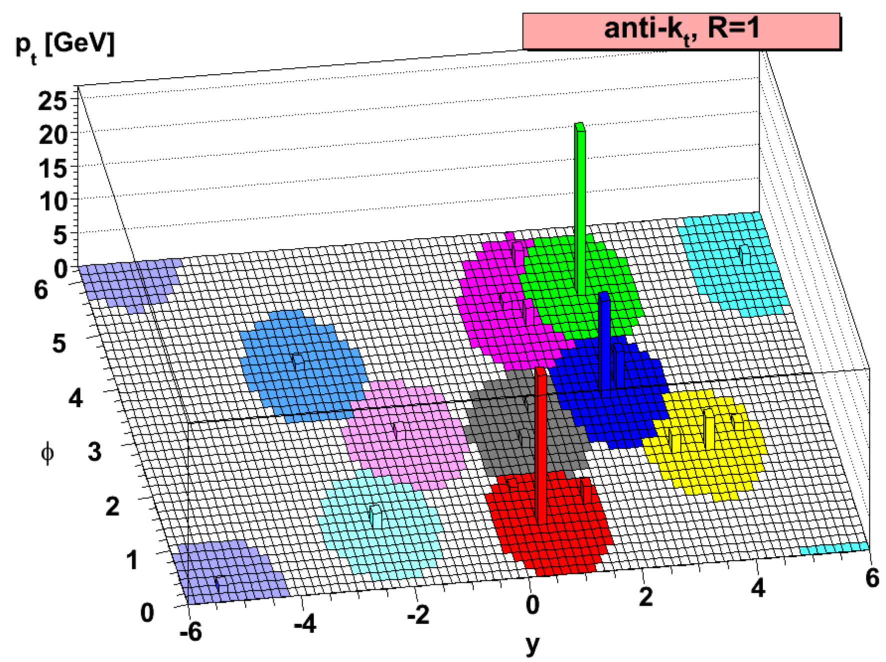
Every 25 nanoseconds at the LHC

T E H M

γ 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 $O(N^3)$

$\Downarrow$

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

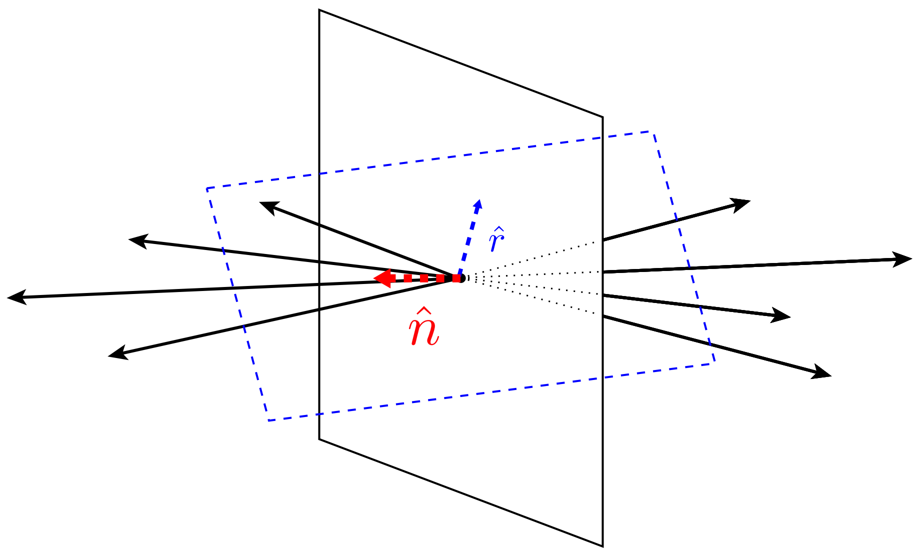
We work really hard to avoid exponentially hard data analysis problems!

[Cacciari, Salam, PLB 2006; Cacciari, Salam, Soyez, JHEP 2008]

Until then, leveraging quantum inspirations!

Even though practical algorithms are currently classical…

Challenge of Data Loading



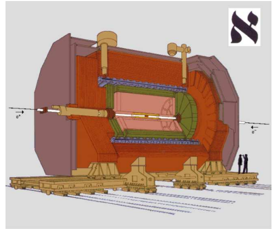
Degeneracy Engineering

Superposition for Graphs

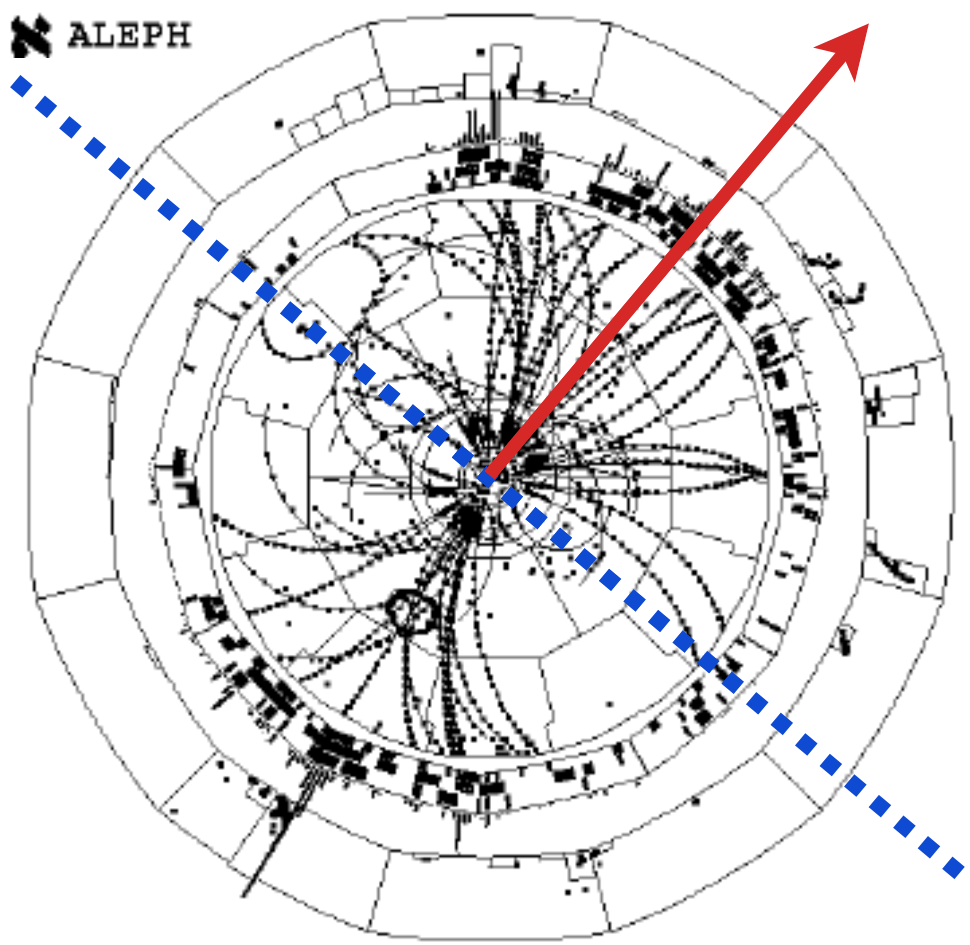
Optimal Transport

if time permits

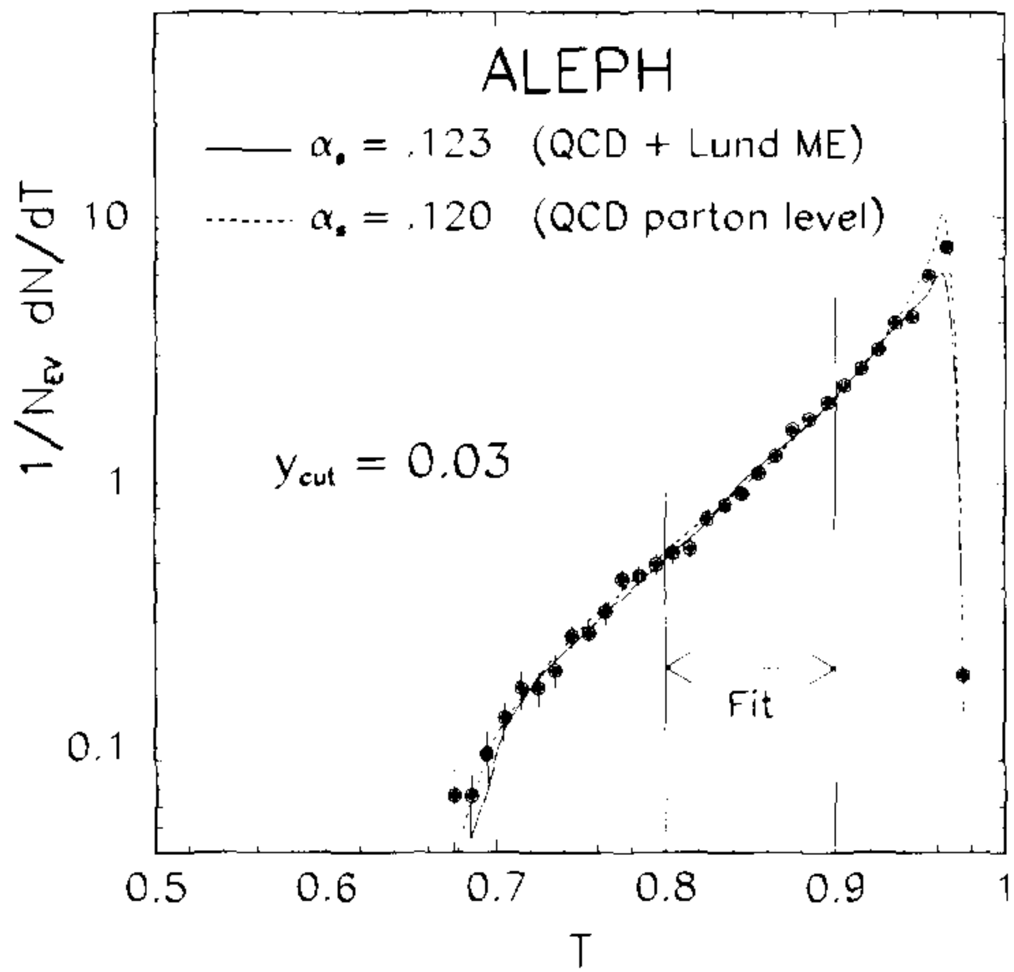
Jet Clustering with Thrust



Classic hemisphere partitioning for e^+e^- colliders

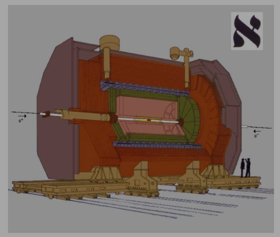


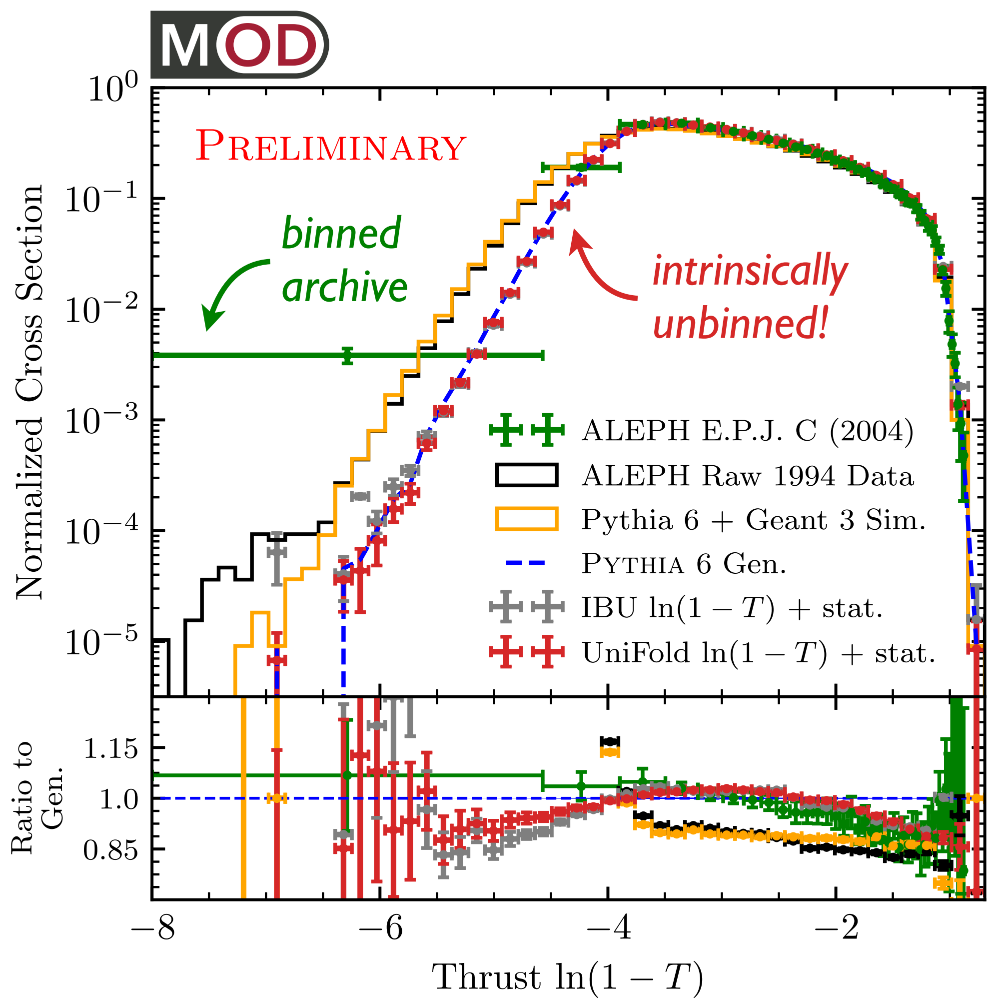
spherical pencil-like



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

Jet Clustering with Thrust



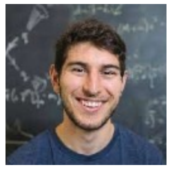


Back to the Future with
ALEPH Archival Data

OmniFold

Multi-dimensional unbinned
detector corrections
via machine learning

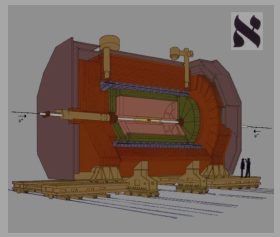
[talk by Badea, ICHEP 2020; cf. ALEPH, EPJC 2004]
[using Andreassen, Komiske, Metodiev, Nachman, JDT, PRL 2020]
[see Badea, Baty, Chang, Innocenti, Maggi, McGinn, Peters, Sheng, JDT, Lee, PRL 2019]
[for unbinned archival strategy see Arratia, et al., arXiv 2021]





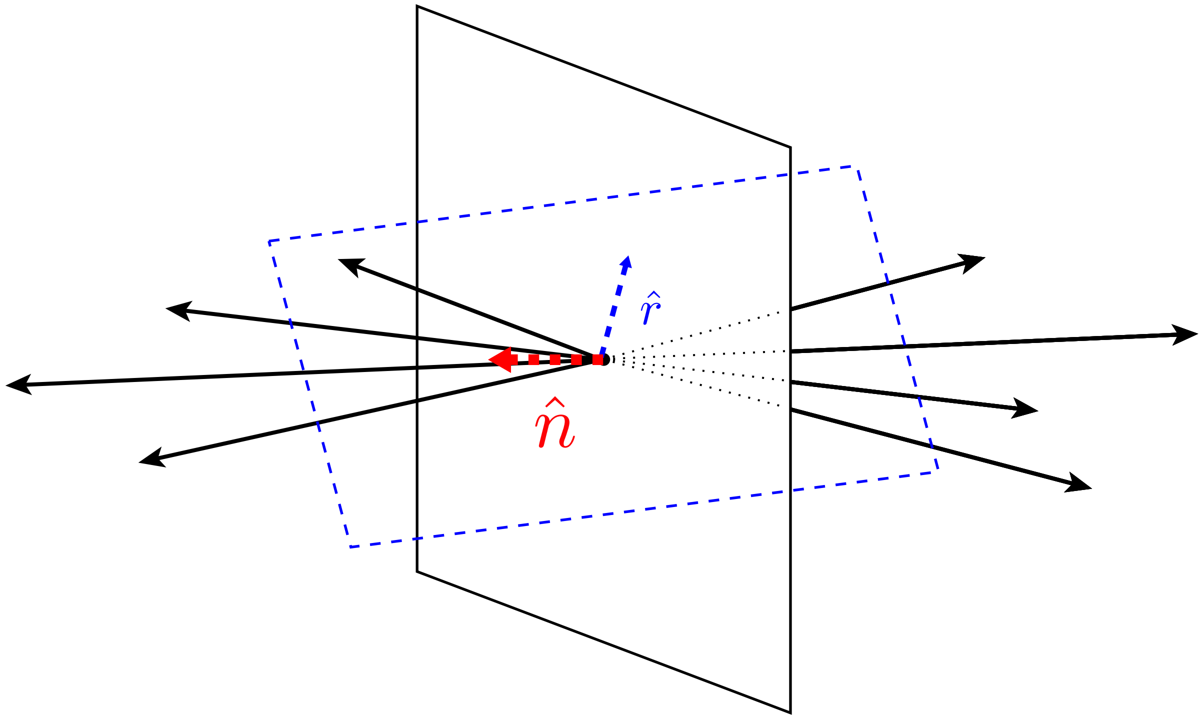

[Brandt, Peyrou, Sosnowski, Wroblewski, PL 1964; Farhi, PRL 1977; ALEPH, PLB 1991]

Jet Clustering with Thrust



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

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



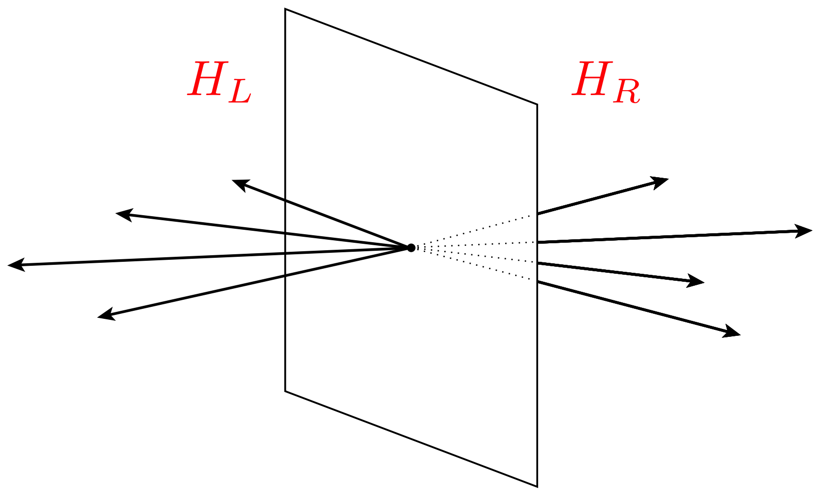
Trick: Recast axis finding as partition finding

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

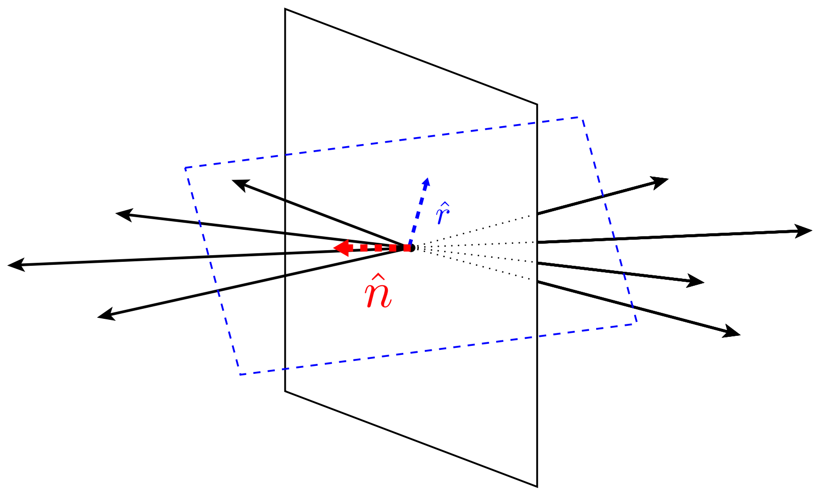
[Yamamoto, JCP 1983; default algorithm in Pythia 8]

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

Quantum Jet Clustering



Dual Formulations



Naive Partitioning: O(2^N)

⇓

QUBO for Quantum Annealing

Key lesson:
Very good classical heuristics

Best Known Classical: O(N^3)

⇓

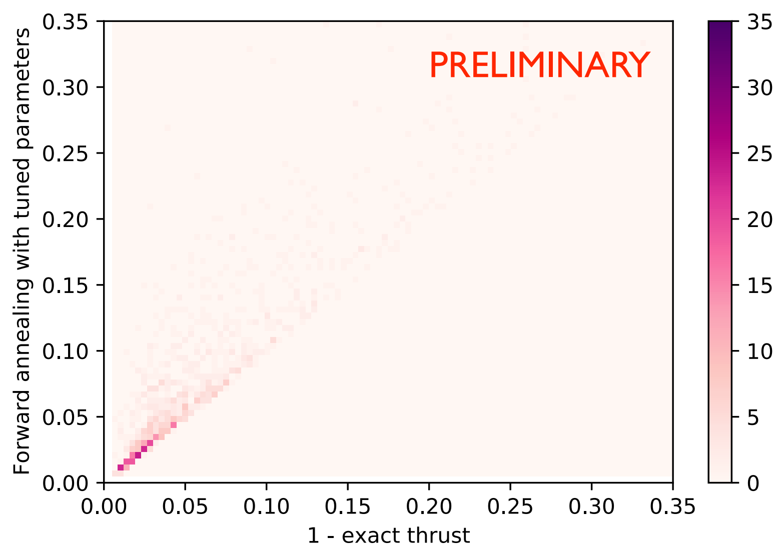
O(N^2) with Grover-style Search

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]

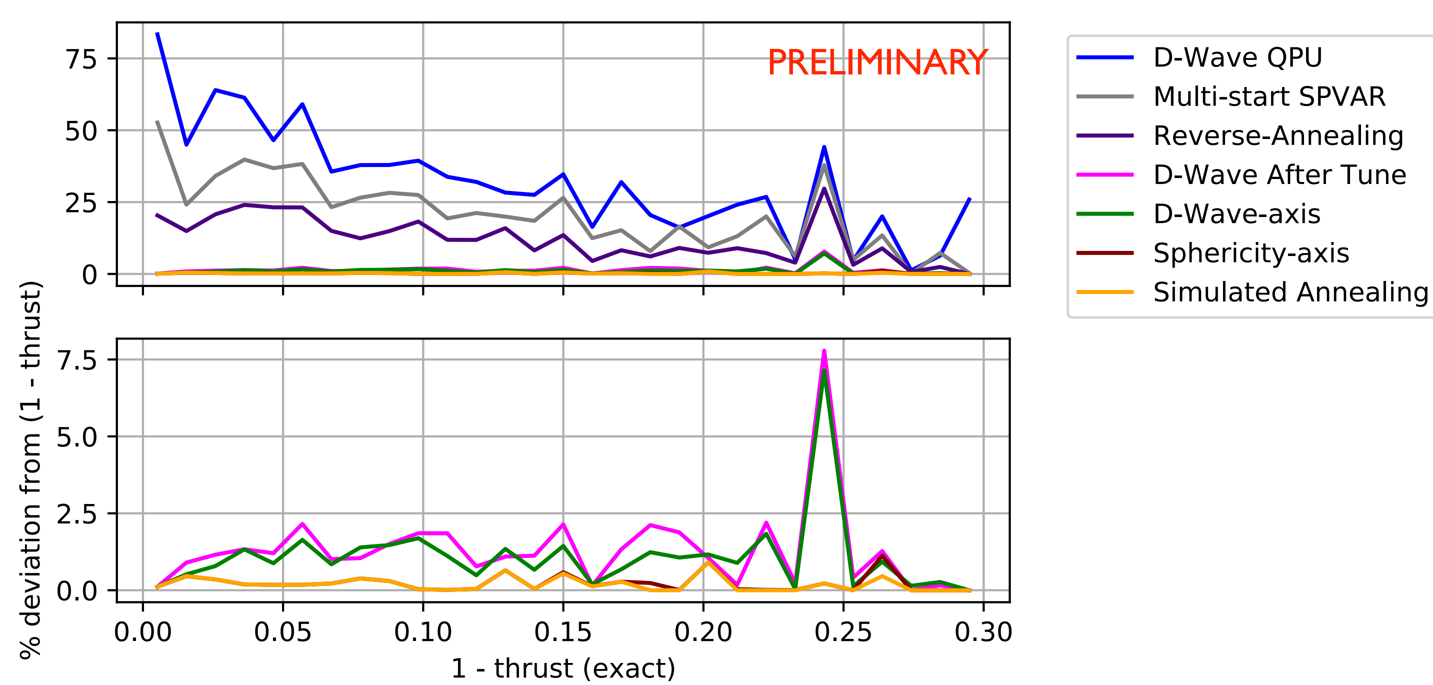
Quantum Annealing for Thrust

D-Wave Advantage can handle O(100) particles



Good correlation for tuned annealing schedule!

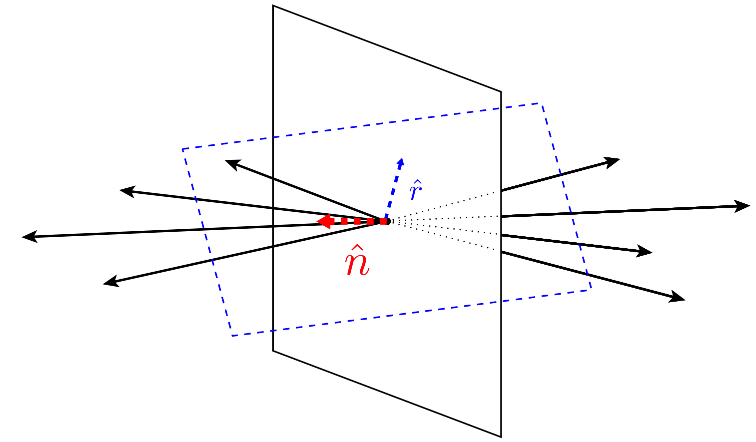
But iterative heuristic does comparably well



[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 $\texttt{curr\_max} = (m, n)$.
2. Compute $\texttt{p\_sum} = \frac{1}{2}\sum_{i=1}^{2N} |\vec{p}_i|$.
3. Set $\texttt{iter\_count} = 0$ and $\texttt{max\_it} = 1$.
4. While $\texttt{iter\_count} < O(N)$:
   (a) While $\texttt{max\_it} < O(N)$:
      i. Prepare the initial state $|\psi_0\rangle = \frac{1}{2N}\sum_{i,j=1}^{2N} |i\rangle\,|j\rangle\,|\vec{0}\rangle\,|\vec{0}\rangle\,|\hat{0}\rangle\,|\vec{0}\rangle\,|0\rangle$.
      ii. Choose $\texttt{grov\_steps}$ uniformly at random from $\{0, 1, ..., \texttt{max\_it} - 1\}$.
      iii. Let $\texttt{iter\_count} = \texttt{iter\_count} + \texttt{grov\_steps}$.
      iv. Repeat $\texttt{grov\_steps}$ times:
         A. Call subroutine $\texttt{COMP\_T}$ 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 $T_{ij} > T_{\texttt{curr\_max}}$ with a phase factor:
         $$|i\rangle\,|j\rangle\,|\vec{0}\rangle\,|\vec{0}\rangle\,|\hat{0}\rangle\,|\vec{0}\rangle\,|T_{ij}\rangle \mapsto (-1)^{\Theta(T_{ij} - T_{\texttt{curr\_max}})}\,|i\rangle\,|j\rangle\,|\vec{0}\rangle\,|\vec{0}\rangle\,|\hat{0}\rangle\,|\vec{0}\rangle\,|T_{ij}\rangle\,.$$
         C. Uncompute the T_{ij} register to obtain state: $(-1)^{\Theta(T_{ij} - T_{\texttt{curr\_max}})}\,|i\rangle\,|j\rangle\,|\vec{0}\rangle\,|\vec{0}\rangle\,|\hat{0}\rangle\,|\vec{0}\rangle\,|0\rangle$.
         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 $T_{k\ell} > T_{\texttt{curr\_max}}$, set $\texttt{curr\_max} = (k, \ell)$ and break.
   (b) Let $\texttt{max\_it} = \mu \times \texttt{max\_it}$, where μ is a constant between 1 and 4/3.
5. Measure the $\{i, j, T_{ij}\}$ registers to obtain $\{k, \ell, T_{k\ell}\}$; if $T_{k\ell} > T_{\texttt{curr\_max}}$, set $\texttt{curr\_max} = (k, \ell)$.

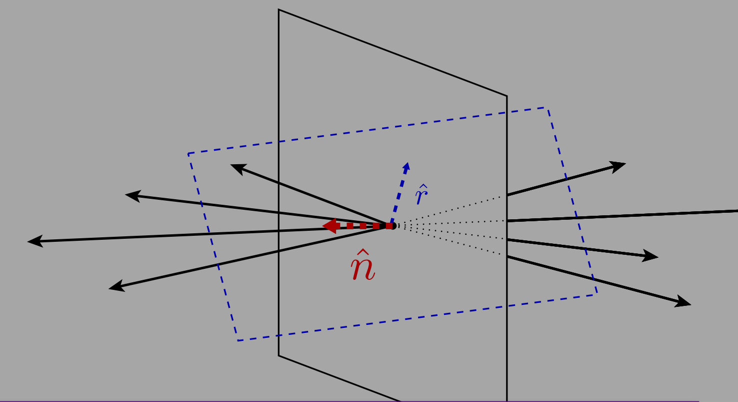
Grover over N^2 partitions in O(N)

How expensive is this?

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

Quantum Search for Thrust

Grover search to find optimal partition



1. Rand
2. Comp
3. Set it
4. While
   (a)

Subroutine COMP_T:

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 $T_{ij} = 2|\vec{P}_{ij}|/\texttt{p\_sum}$:

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

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

And this?

Grover over N^2 partitions in O(N)

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

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 $T_{k\ell} > T_{\texttt{curr\_max}}$, set `curr_max` $= (k, \ell)$ and break.

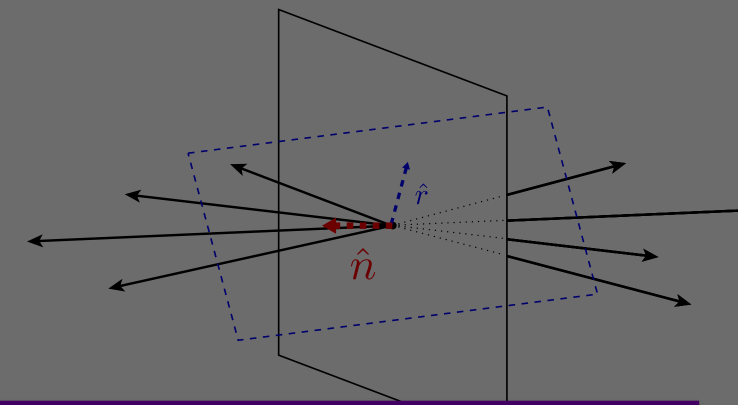
(b) Let `max_it` $= \mu \times$ `max_it`, where μ is a constant between 1 and 4/3.

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

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

Quantum Search for Thrust

Grover search to find optimal partition



1. Rand
2. Comp
3. Set it
4. While

   (a)

Subroutine `COMP_T`:

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 $\hat{r}_{ij} = (\vec{p}_i \times \vec{p}_j)/|\vec{p}_i \times \vec{p}_j|$:

3. Apply SU ... entum $\vec{P}_{ij}$:

4. Calculate

5. Uncompu

And this?

Grover over N^2 partitions in O(N)

C. Uncomp

D. Reflect

v. Measure the ... ak.

(b) Let `max_it` $= \mu$

5. Measure the $\{i, j, T_{ij}\}$

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]

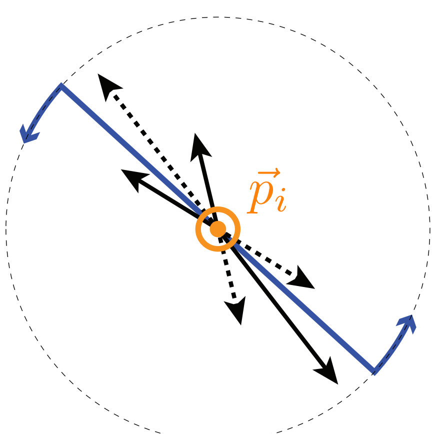
[Wei, Naik, Harrow, JDT, PRD 2020]



Final Scorecard for Quantum Thrust

Quantum search gives O(N²) ≪ O(N³)!

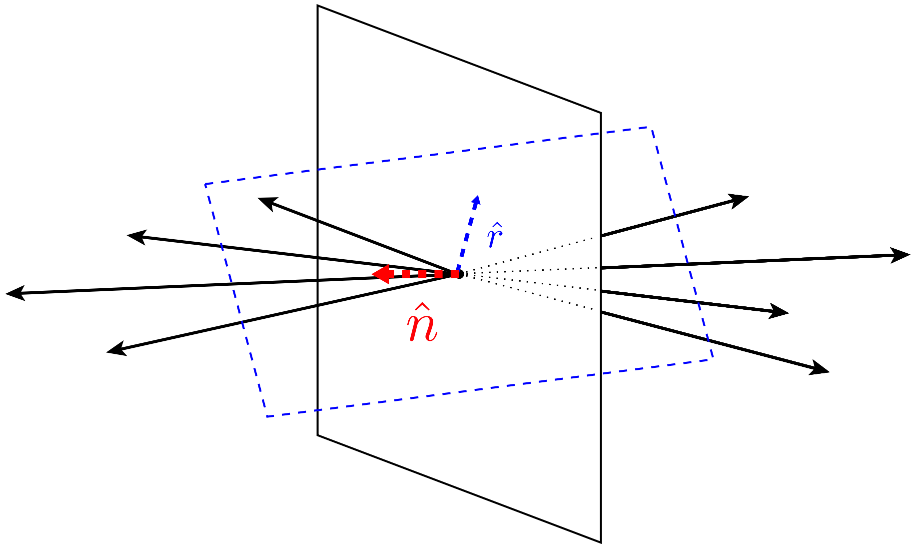
Implementation	Time Usage	Qubit Usage
Classical [2]	$O(N^3)$	—
Classical with Sort (using [3])	$O(N^2 \log N)$	
Classical with Parallel Sort	$O(N \log N)$	—
Quantum Annealing	Gap Dependent	$O(N)$
Quantum Search: Sequential Model	$O(N^2)$	$O(\log N)$
Quantum Search: Parallel Model	$O(N \log N)$	$O(N \log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



But we found new O(N² log N) algorithm using classical sort…

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





Quantum Inspiration:

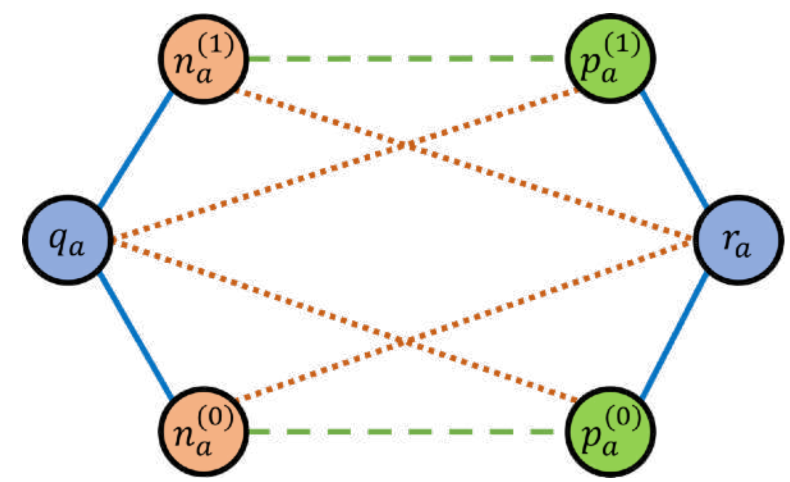
Solving jet optimization using annealing or Grover search

Classical Development:

Improved $O(N^2 \log N)$ thrust algorithm with classical sort

Challenge of Data Loading

Degeneracy Engineering

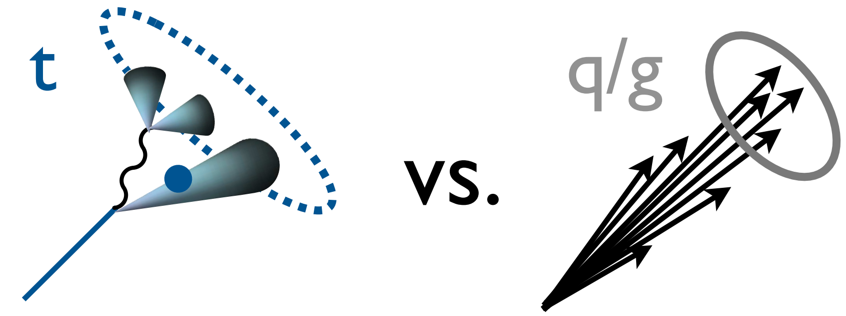


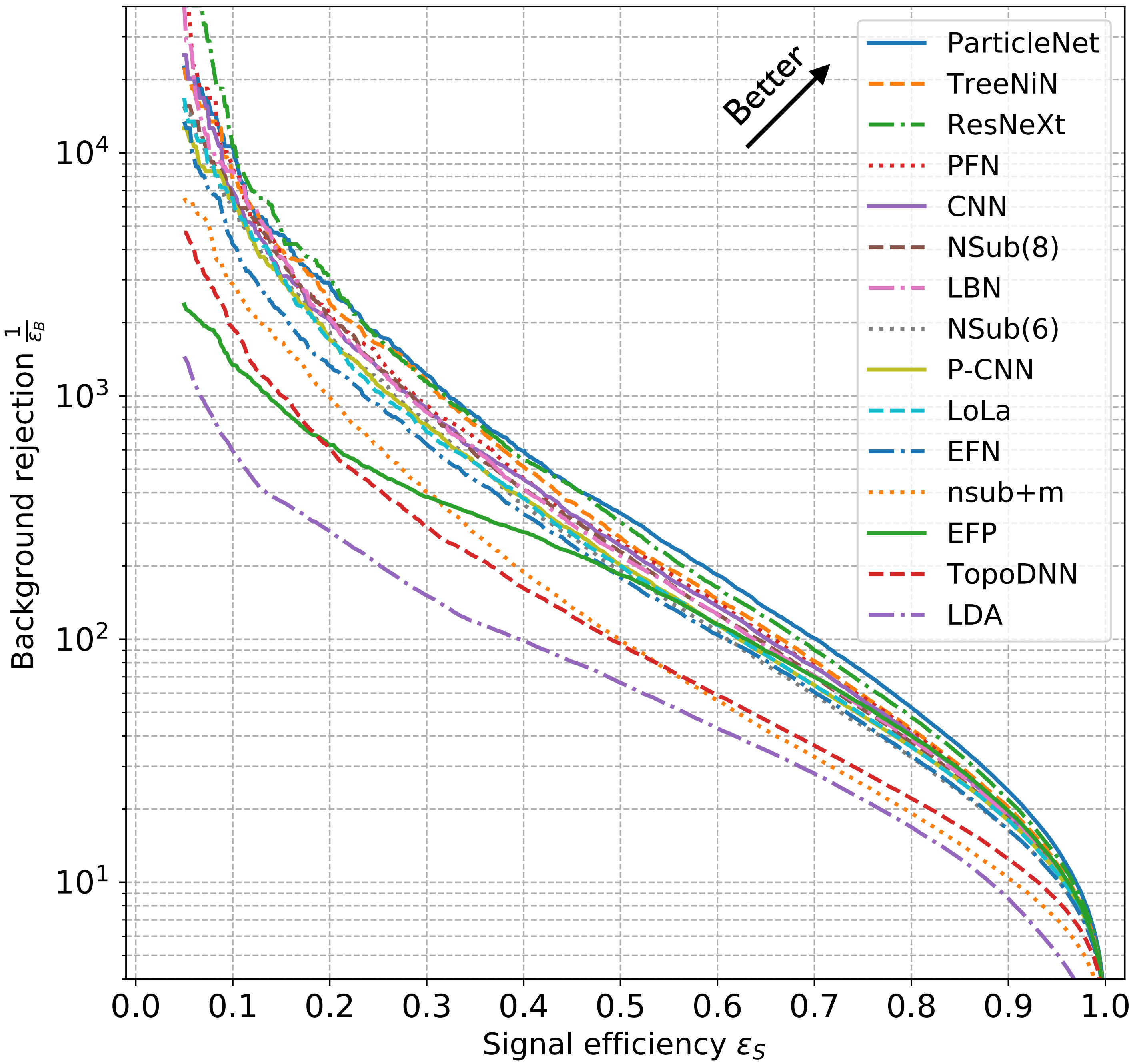
Superposition for Graphs

Optimal Transport

if time permits

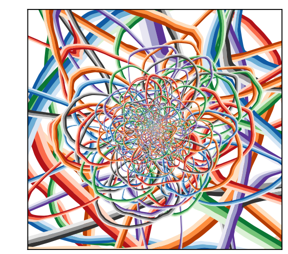
Rise of the Machines?



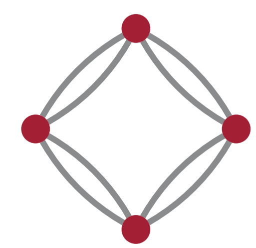


1,460,000 parameters

85,000 parameters
Energy Flow Networks



1,000 parameters
Energy Flow Polynomials



[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]

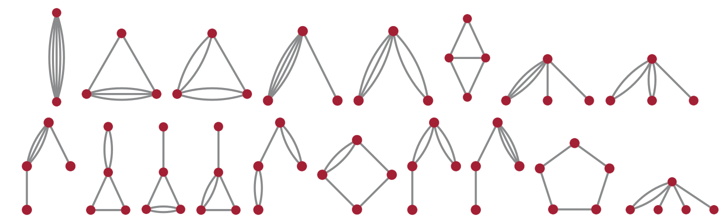


Energy Flow Polynomials for Jet Substructure

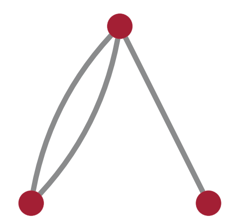
Case study for sparse linear regression

Linear basis for IRC-safe collider observables:

$$\mathcal{S} = \sum_G s_G \, \mathrm{EFP}_G$$



(more about IRC safety later)

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_2-Norm (Ridge): Not sparse

L_1-Norm (Lasso): Biased answers

L_0-Norm: NP-hard $\Rightarrow$ Annealing?

[Komiske, Metodiev, JDT, JHEP 2018]

Sparse Linear Regression

Standard Loss Function $$L_{\mathrm{MSE}} = \sum_{s \in \mathcal{S}} \Big(y_s - h(\vec{x}_s) \Big)^2$$

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 $$L = L_{\mathrm{MSE}} + \lambda \, R$$

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

L_0-Norm (p = 0) not of quadratic form (i.e. Ising/QUBO)…

Sparse Linear Regression for Annealing

Standard Loss Function $$L_{\text{MSE}} = \sum_{s \in \mathcal{S}} \Big(y_s - h(\vec{x}_s) \Big)^2$$

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

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

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

Standard Regularization
$$L = L_{\rm MSE} + \lambda \, R$$

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

PRELIMINARY

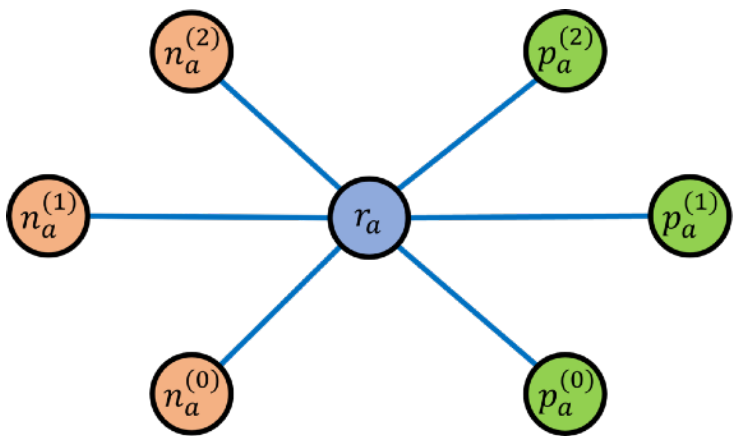
$$+ \, r_a + (1 - r_a + 2 q_a) \sum_{i=1}^{M} n_a^{(i)} - 2 \sum_{i=1}^{M} p_a^{(i)} \, n_a^{(i)}$$

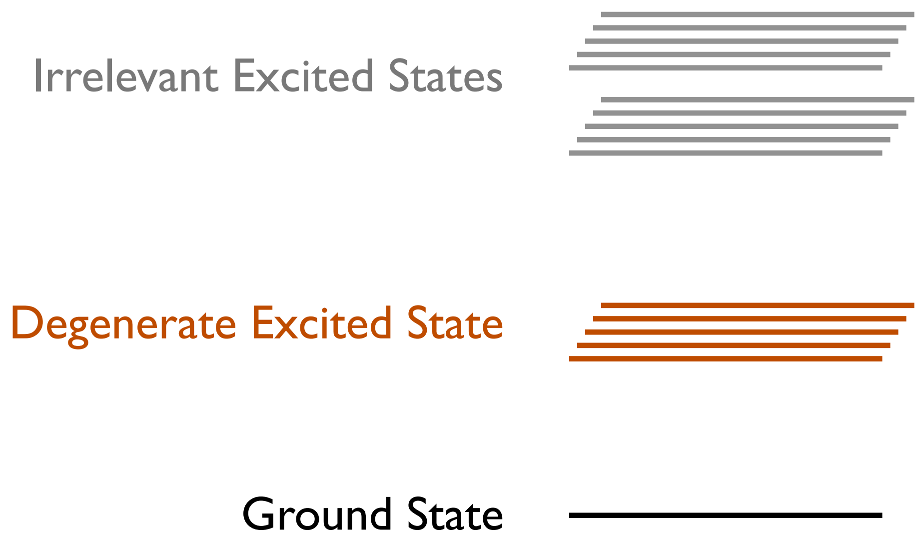
Key: Degeneracy Engineering

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

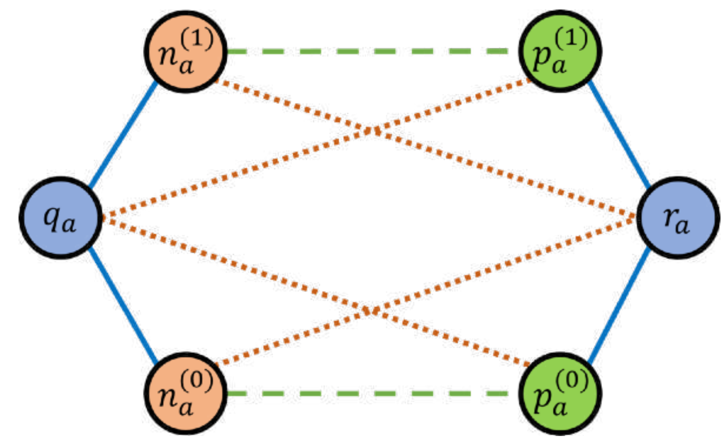
Degeneracy Engineering

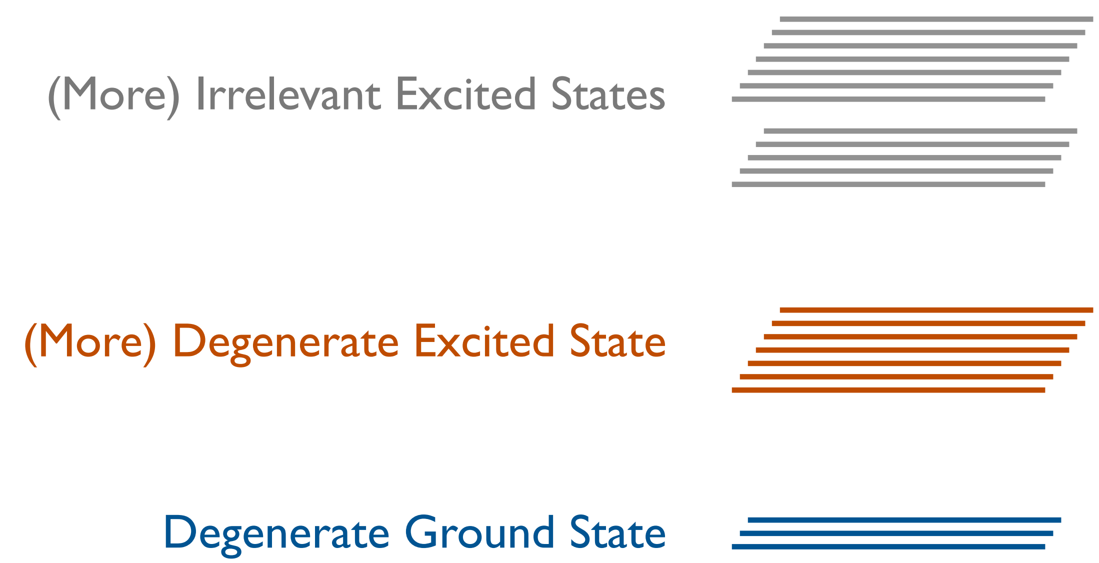
Single Latent Bit





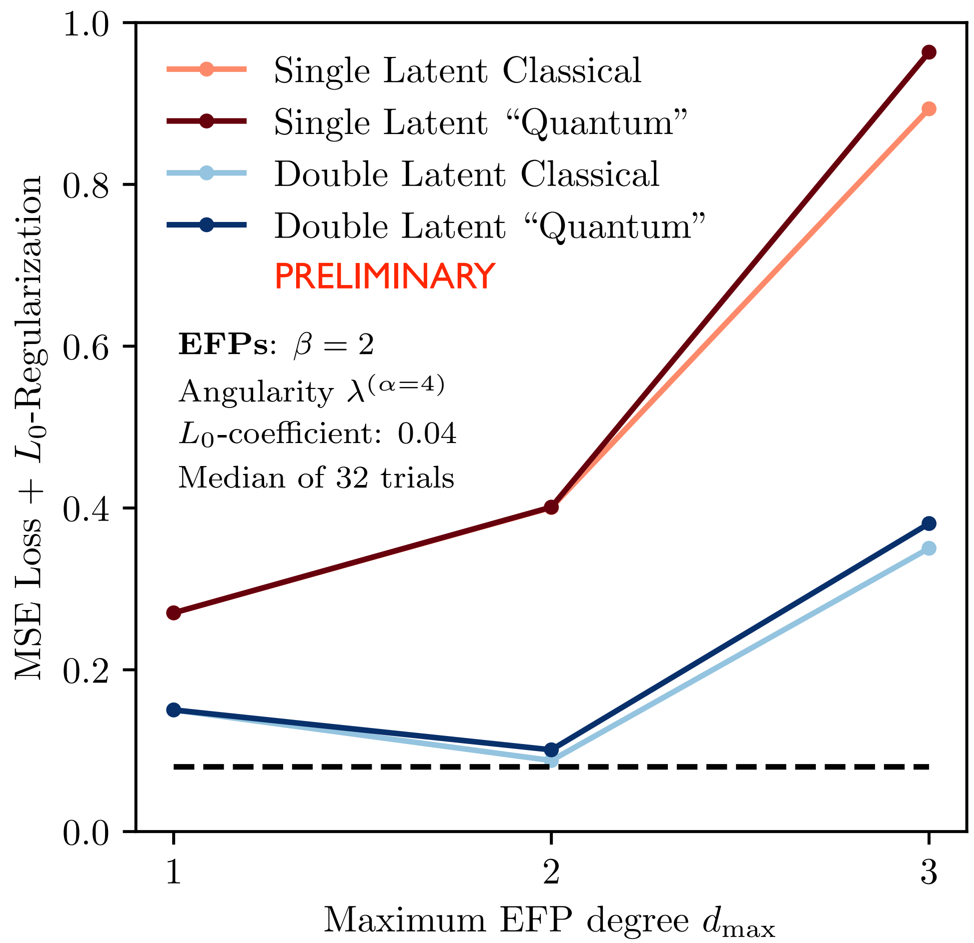
Double Latent Bit





More efficient as relative degeneracy of ground state increases

Degeneracy Engineering



Single

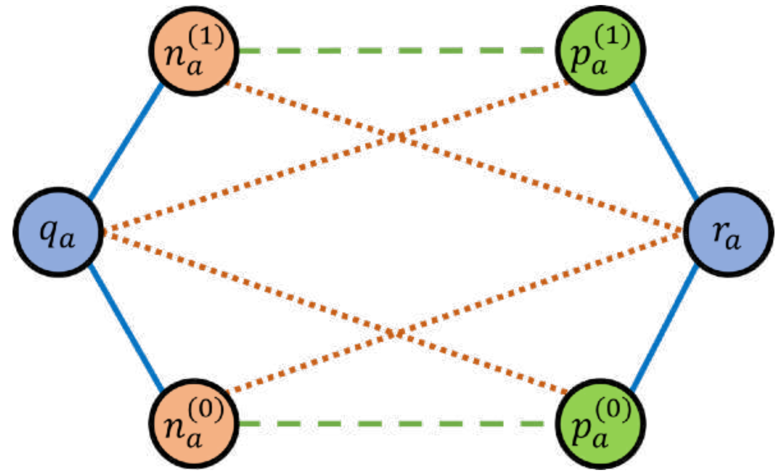
Double

Bigger improvement from latent encoding than classical vs. "quantum" (PIMC)

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




More efficient as relative degeneracy of ground state increases



Quantum Inspiration:

Finding sparse regression solutions through annealing

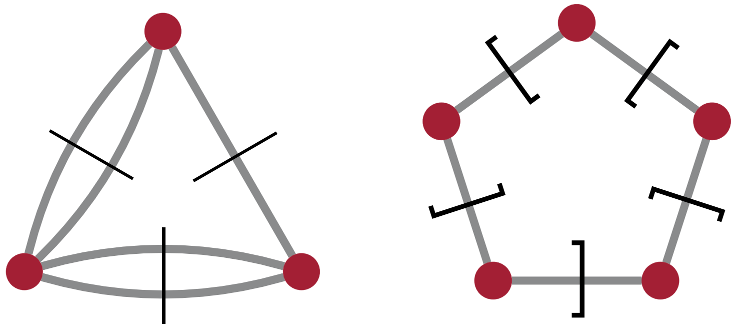
Classical Development:

Improved quadratic loss landscape for L_0-norm regularization

Challenge of Data Loading

Degeneracy Engineering

Superposition for Graphs

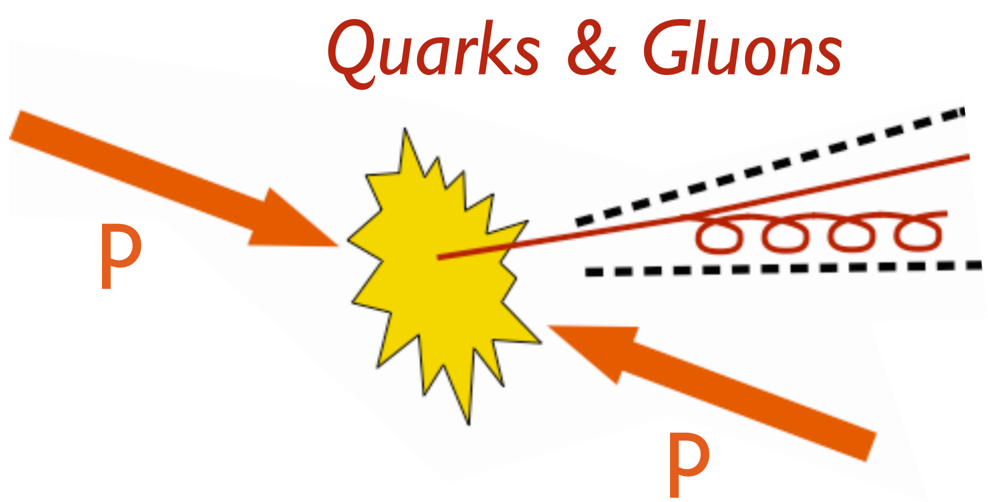


Optimal Transport

if time permits

Energy Flow Representation

Respects infrared and collinear safety

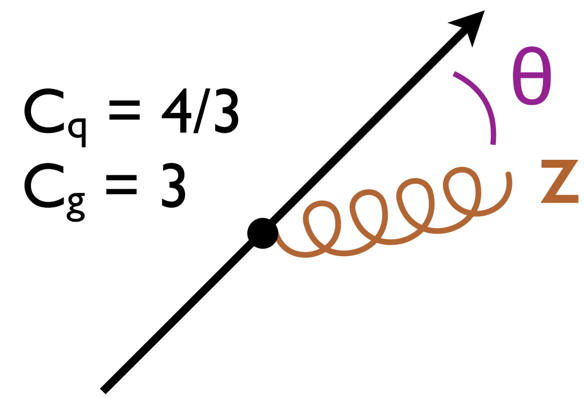


Conceptual challenge:
Splitting obscures quantum coherence,
complicates quantum encoding

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

Altarelli-Parisi Splitting

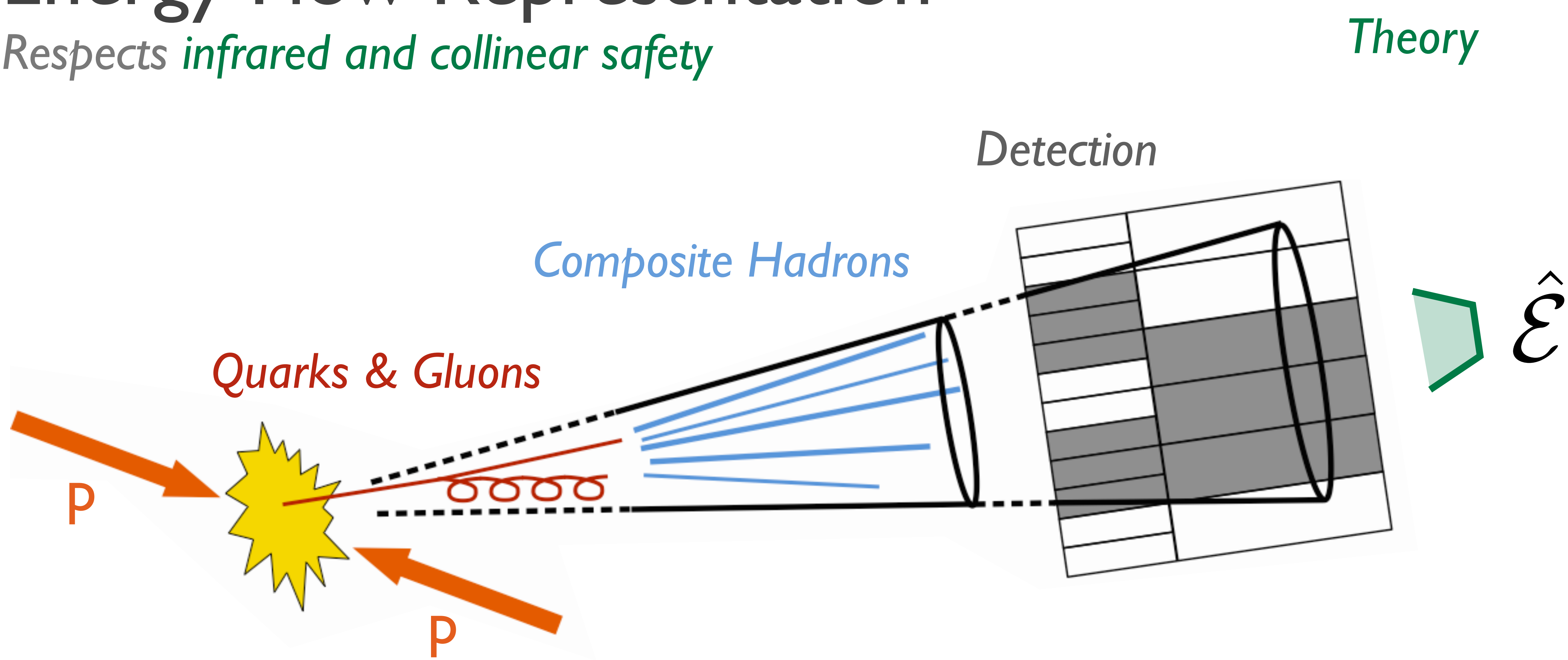
Core prediction of QCD



$$\mathrm{d}P_{i\to ig} \simeq \frac{2\alpha_s}{\pi} C_i \underbrace{\frac{\mathrm{d}\theta}{\theta}}_{\text{Collinear}} \underbrace{\frac{\mathrm{d}z}{z}}_{\text{Soft}}$$

Energy Flow Representation

Respects infrared and collinear safety



Energy Flow:

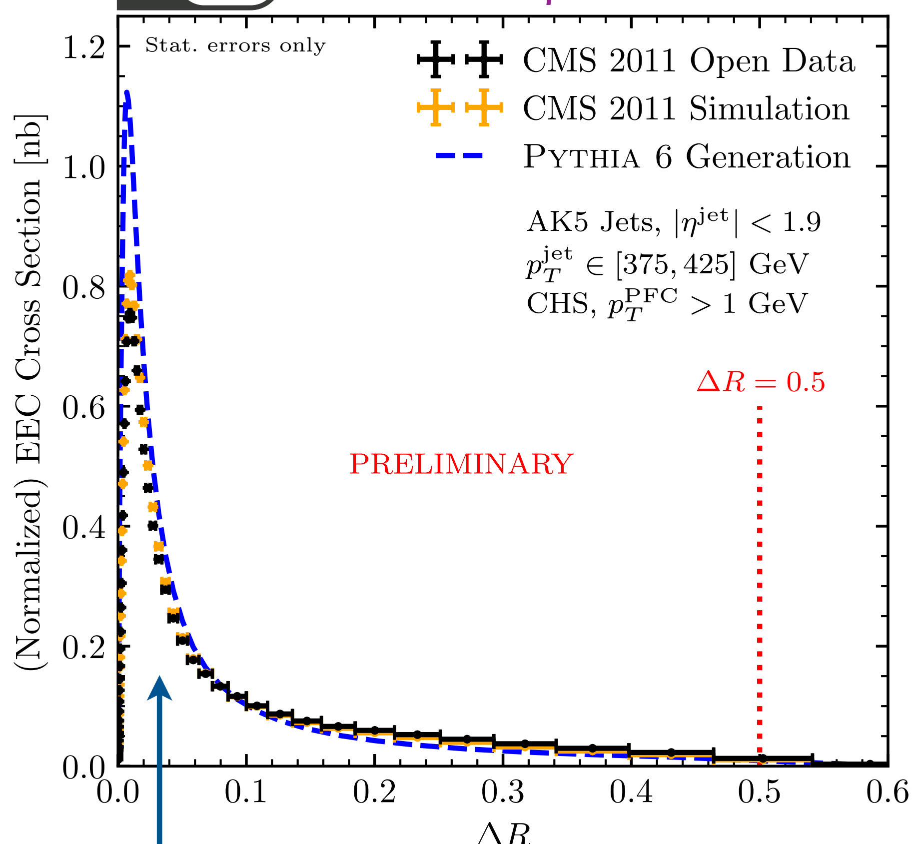
Robust to hadronization and detector effects
Well-defined for massless gauge theories

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

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

QCD Phase Transition in Jets?

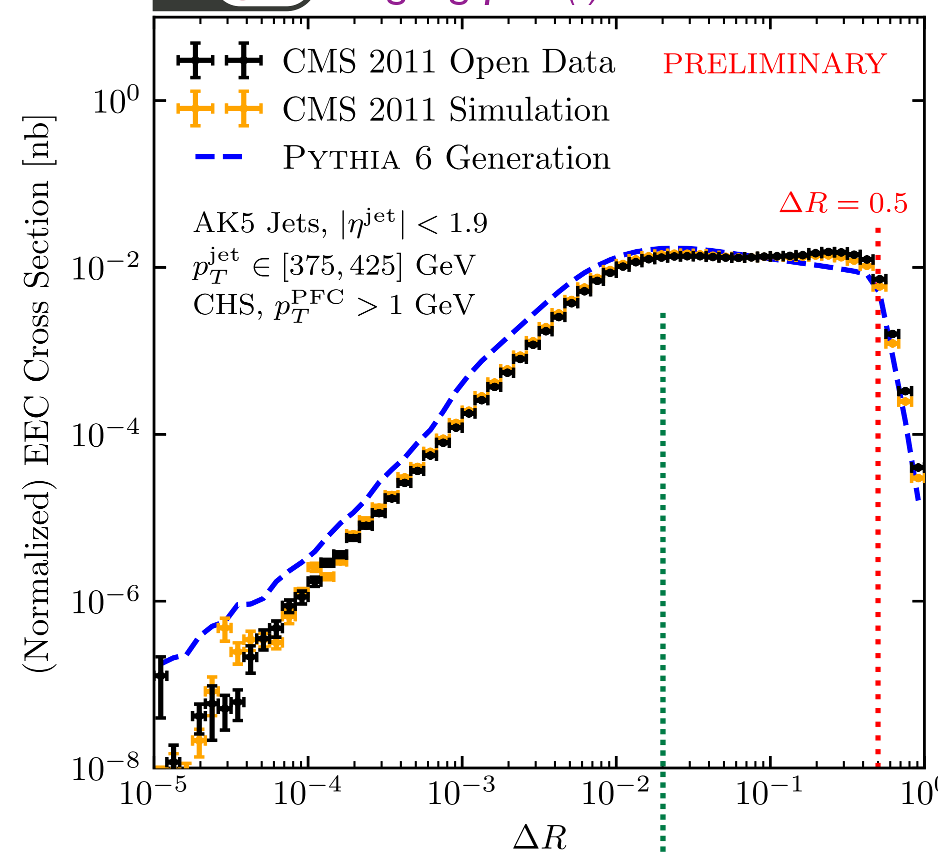
Linear-linear plot



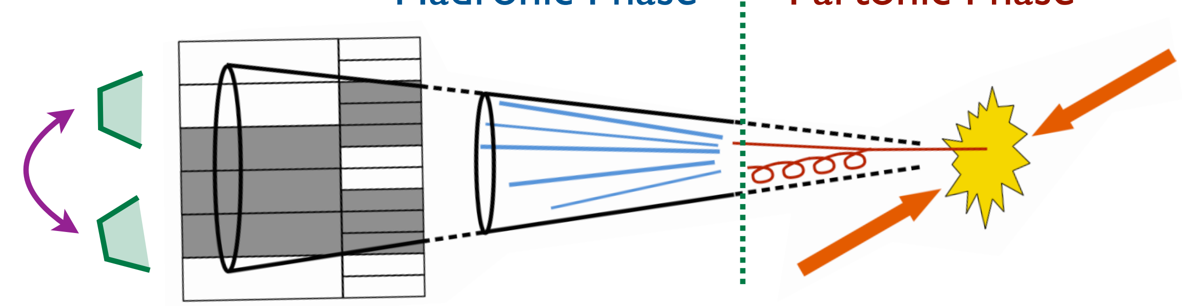
Are we learning something about small angle limit of QCD?

First Jet EEC Plot from the LHC (!)

Log-log plot (!)



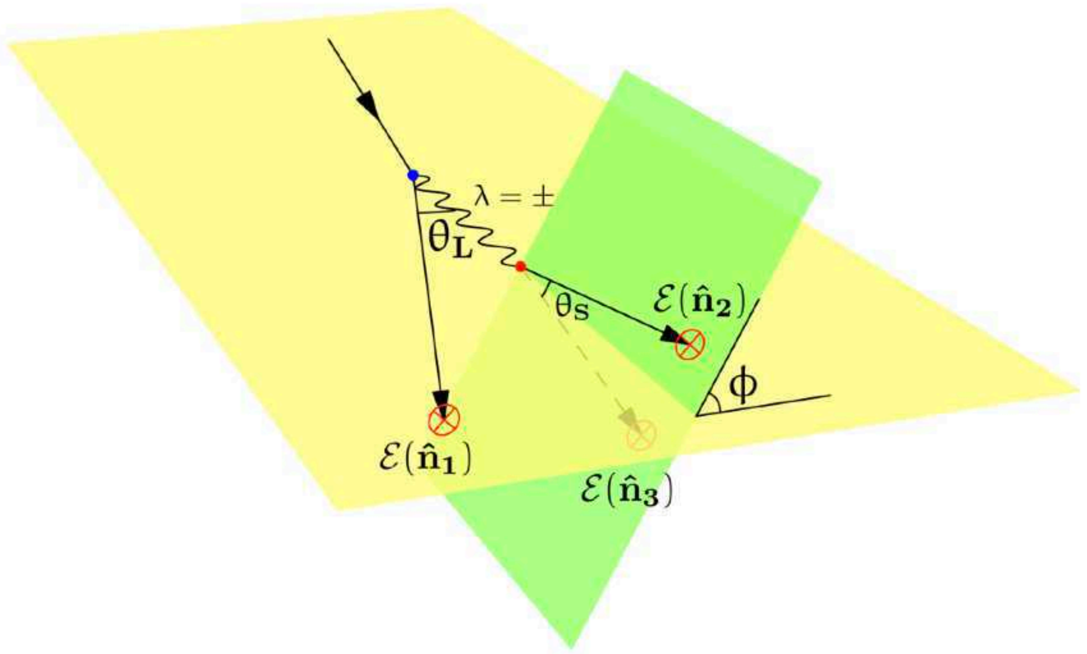
Hadronic Phase ← → Partonic Phase

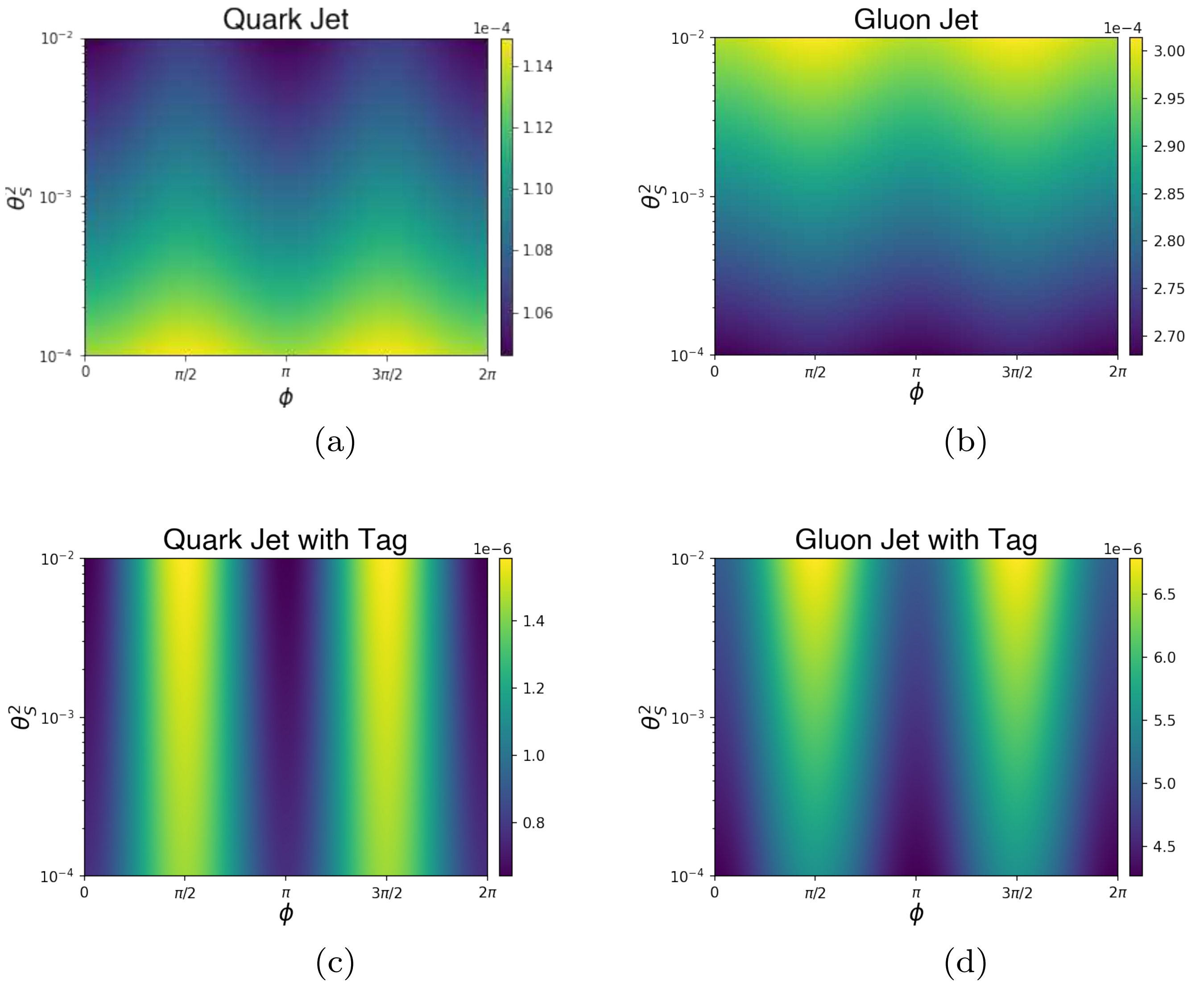




[Komiske, Moult, JDT, Zhu, arXiv 2022; see talks by Moult, BOOST 2019, BOOST 2020]

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

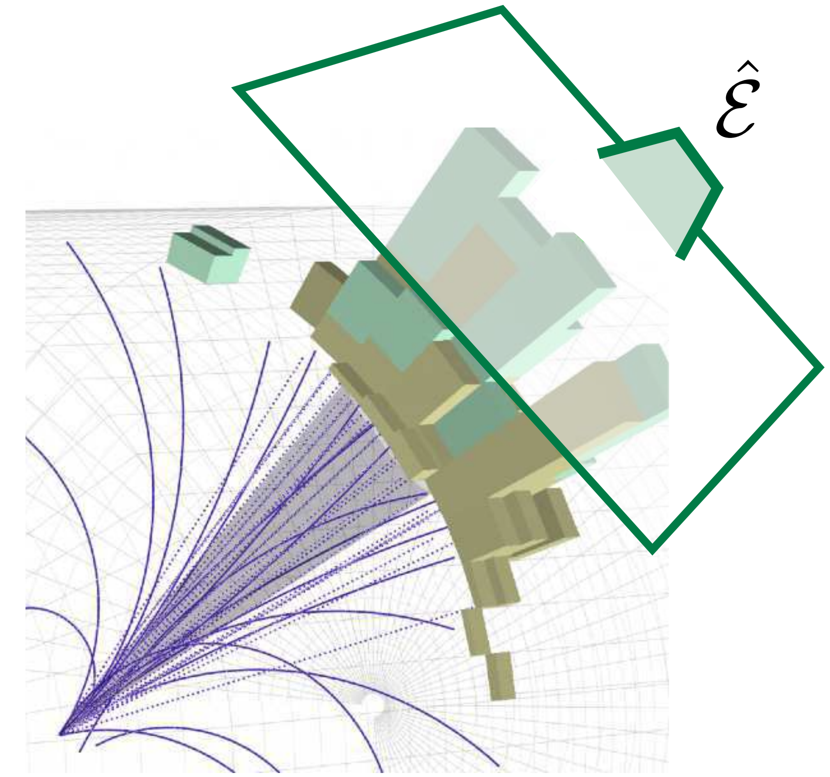
- Energy-Weighted Directions

$$\vec{p} = \{E, \underbrace{\hat{n}_x, \hat{n}_y, \hat{n}_z}_{\text{Direction}}\}$$

Energy

Direction

(suppressing "unsafe" charge/flavor information)

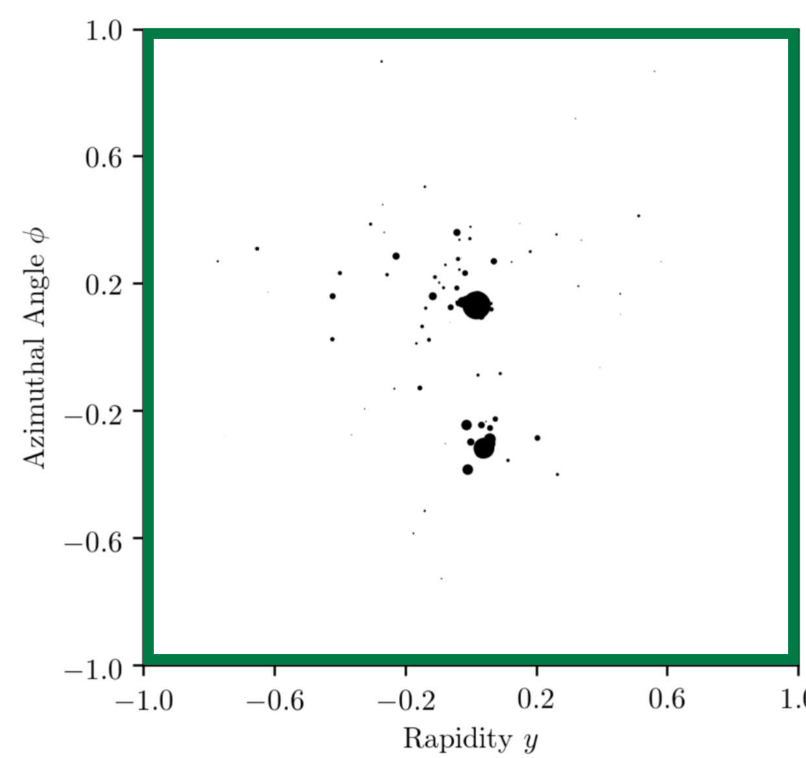


- Equivalently: Energy Density

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

Energy

Direction



Quantum Loading of Point Clouds?

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

$$U_{\textsc{Lookup}} |i\rangle |\vec{0}\rangle = U_{\textsc{Lookup}} |i\rangle |\vec{p}_i\rangle$$

M^2 pairs also takes O(M) quantum

$$U_{\textsc{Lookup}} |i\rangle |\vec{0}\rangle |j\rangle |\vec{0}\rangle = U_{\textsc{Lookup}} |i\rangle |\vec{p}_i\rangle |j\rangle |\vec{p}_j\rangle$$

M^3 triplets also takes O(M) quantum

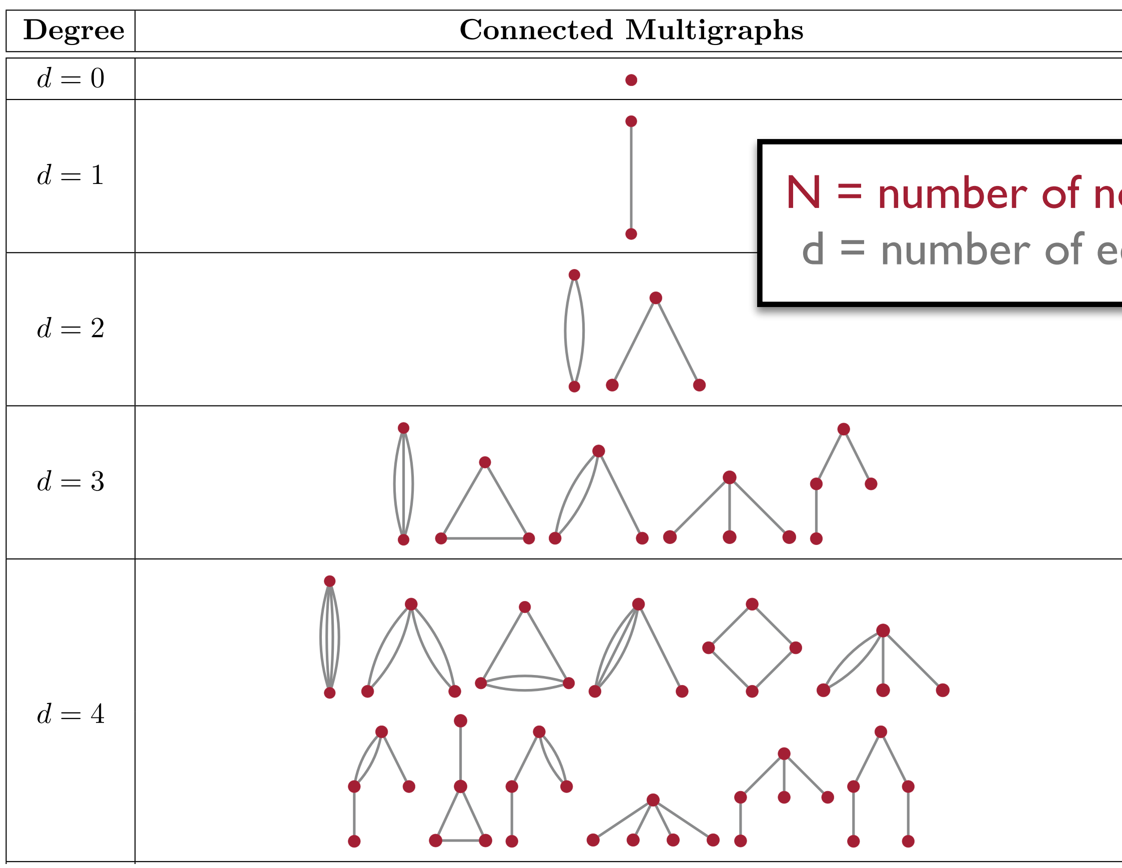
$$U_{\textsc{Lookup}} |i\rangle |\vec{0}\rangle |j\rangle |\vec{0}\rangle |k\rangle |\vec{0}\rangle = U_{\textsc{Lookup}} |i\rangle |\vec{p}_i\rangle |j\rangle |\vec{p}_j\rangle |k\rangle |\vec{p}_k\rangle$$

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)



N = number of nodes
d = number of edges

Cheaper at small d with variable elimination

Enumerating EFPs is combinatorial challenge

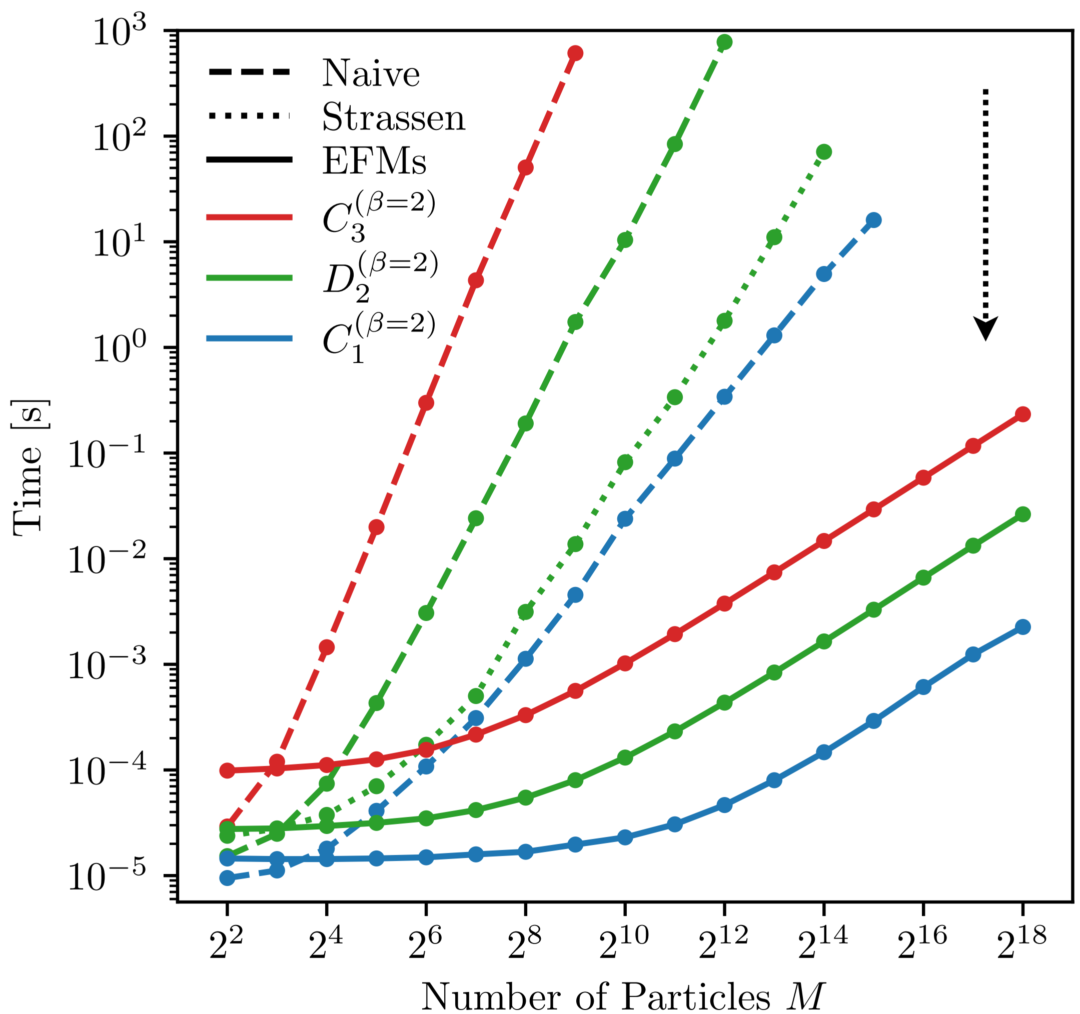
	Leafless Multigraphs	
	Connected	All
Edges d	A307317 [13]	A307316 [14]
1	0	0
2	1	1
3	2	2
4	4	5
5	9	11
6	26	34
7	68	87
8	217	279
9	**718**	**897**
10	**2 553**	**3 129**
11	**9 574**	**11 458**
12	**38 005**	**44 576**
13	**157 306**	**181 071**
14	**679 682**	**770 237**
15	**3 047 699**	**3 407 332**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

EFPs are generically linearly dependent

Is there classical analog to quantum superposition?

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

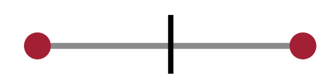
Combinatorics of Energy Flow Polynomials



Yes, if you have "Hilbert space"!

O(M^N) ⇒ O(M) for β=2 EFPs

Simplest example is C_1 ≈ jet mass:



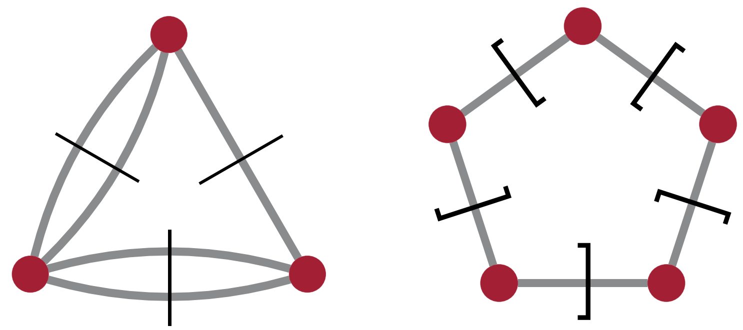
$$\sum_{i=1}^{M}\sum_{j=1}^{M} p_i \cdot p_j$$ O(M^2) vs. O(M) $$\left(\sum_{i=1}^{M} p_i^\mu\right)^2$$

Trick: edges can be expressed as inner products

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

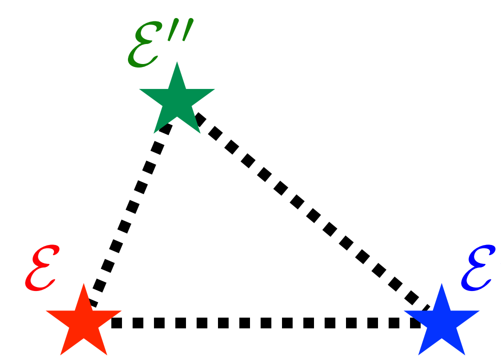
Challenge of Data Loading

Degeneracy Engineering

Superposition for Graphs

Optimal Transport

if time permits



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…

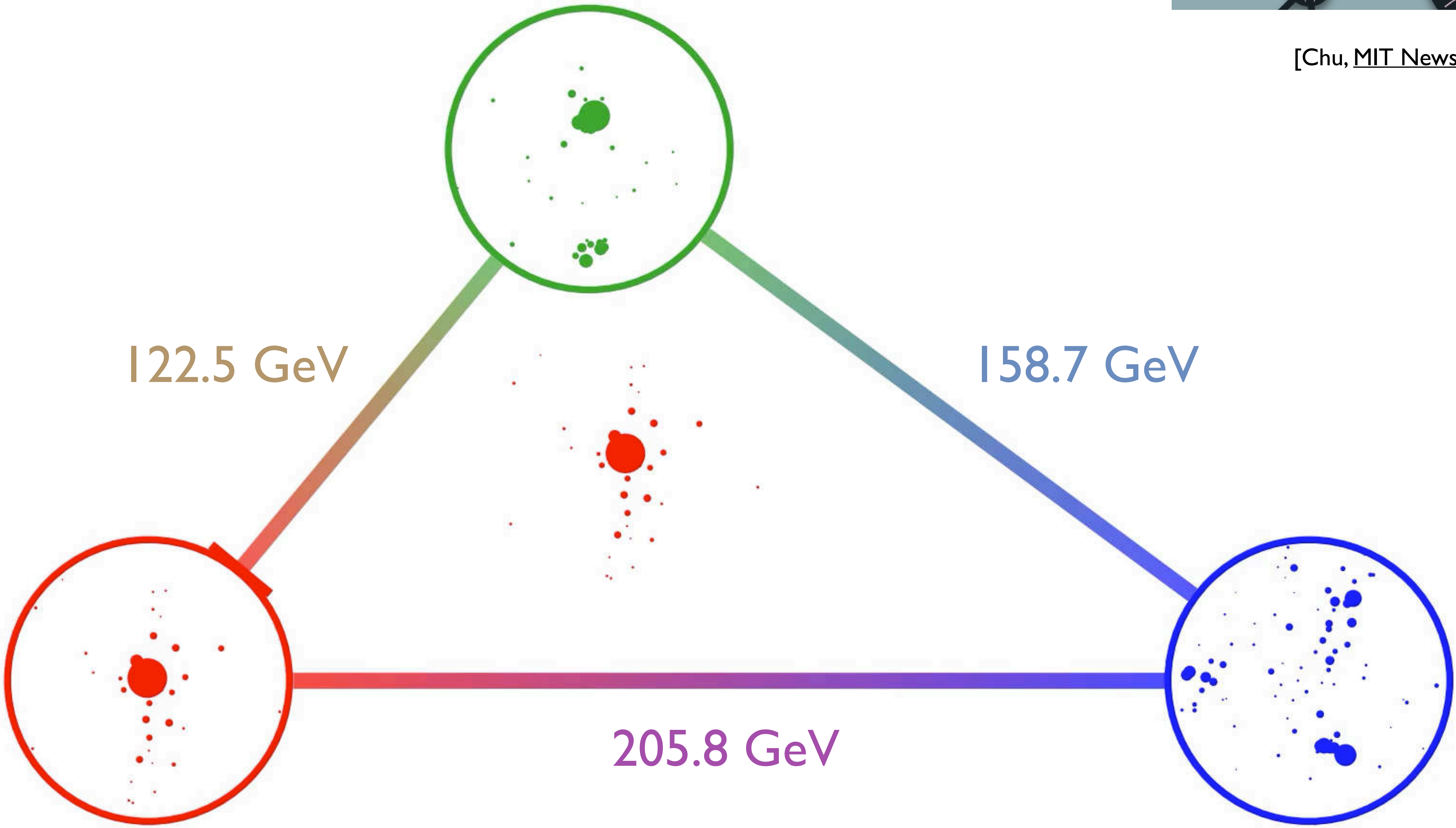
…but I am ready to look beyond $O(N_{event})$ histograms!

Disclaimer: Original motivation was different
How can we compress classical data so it fits on near-term quantum devices?

Graph of O(N²) Event Pairs

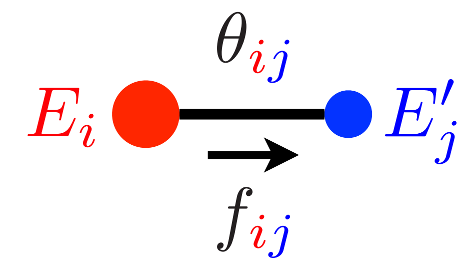
Inspired by Earth Mover's Distance (a.k.a. Wasserstein metric)

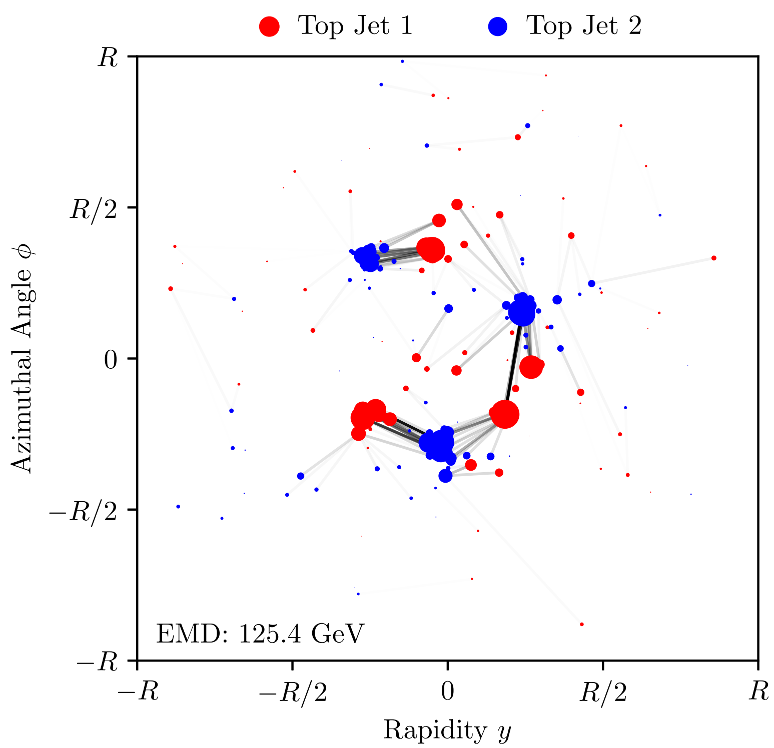
[Chu, MIT News July 2019]



[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; Vaseršteĭn, 1969; Peleg, Werman, Rom, IEEE 1989; Rubner, Tomasi, Guibas, ICCV 1998, ICJV 2000]

The Energy Mover's Distance

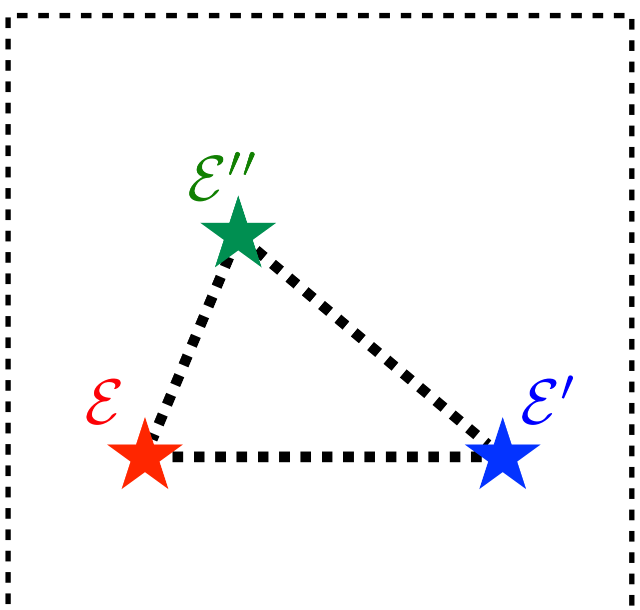




Optimal transport between energy flows…

$$\mathrm{EMD}(\mathcal{E}, \mathcal{E}') = \underbrace{\min_{\{f\}} \sum_i \sum_j f_{ij} \frac{\theta_{ij}}{R}}_{\text{Cost to move energy}} + \underbrace{\left| \sum_i E_i - \sum_j E'_j \right|}_{\text{Cost to create energy}}$$

in GeV



…defines a metric on the space of events

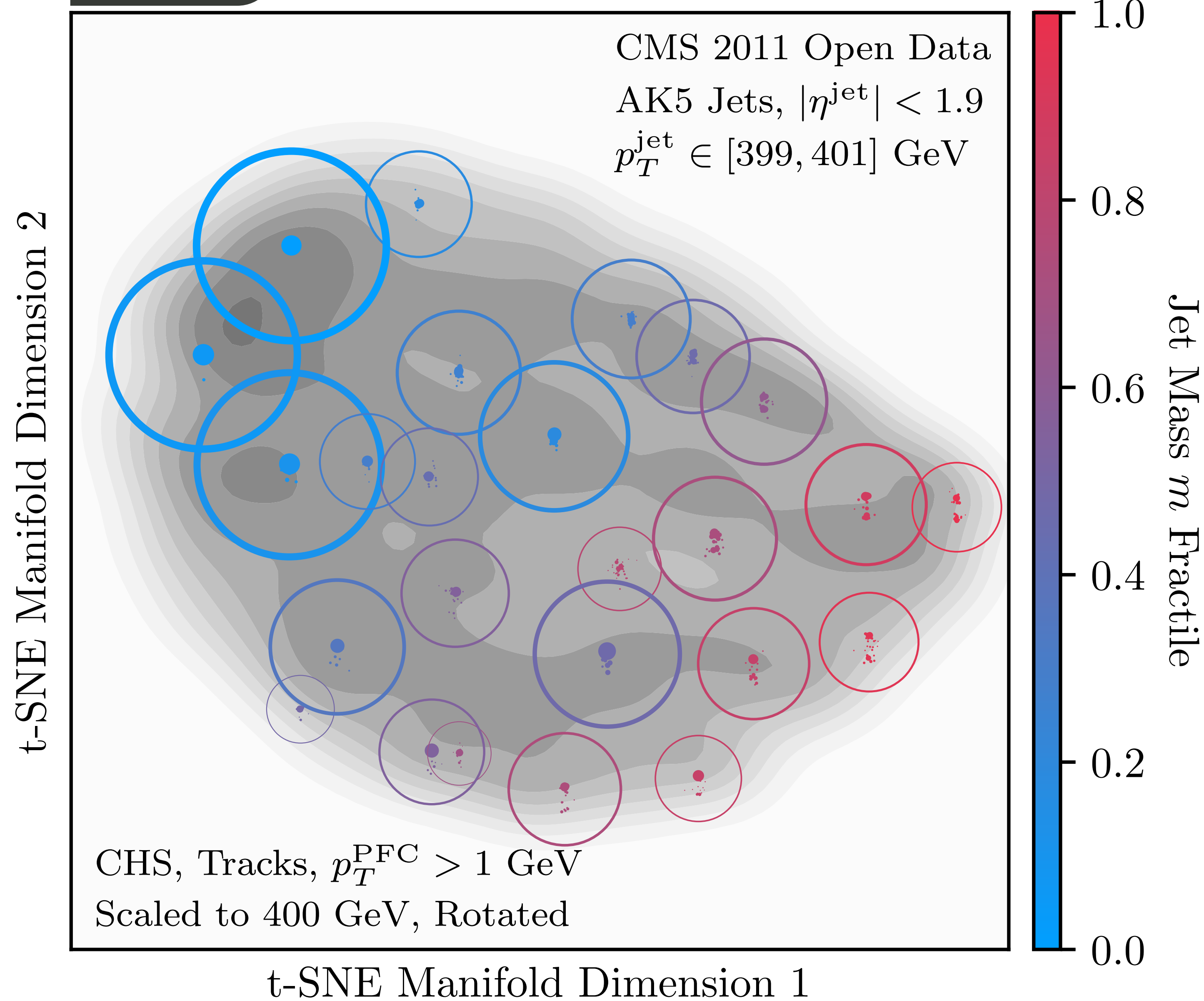
$$0 \leq \mathrm{EMD}(\mathcal{E}, \mathcal{E}') \leq \mathrm{EMD}(\mathcal{E}, \mathcal{E}'') + \mathrm{EMD}(\mathcal{E}', \mathcal{E}'')$$

(assuming R ≥ θ_{max}/2, i.e. R ≥ jet radius for conical jets)

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

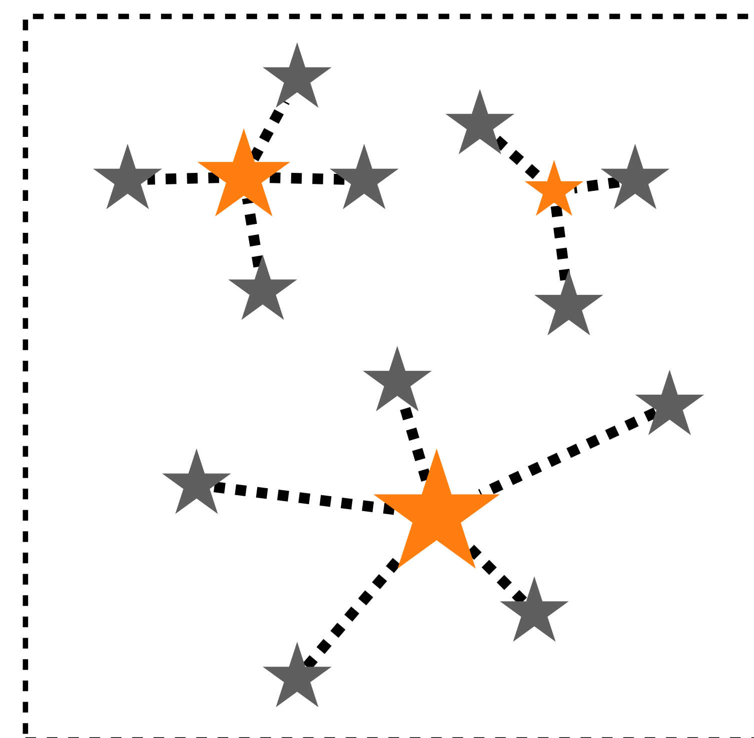
Most Representative Jets

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

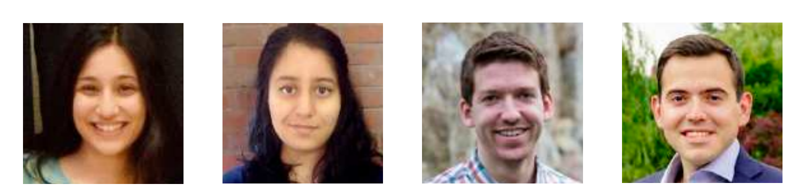


k-medoids

Arranged via t-SNE

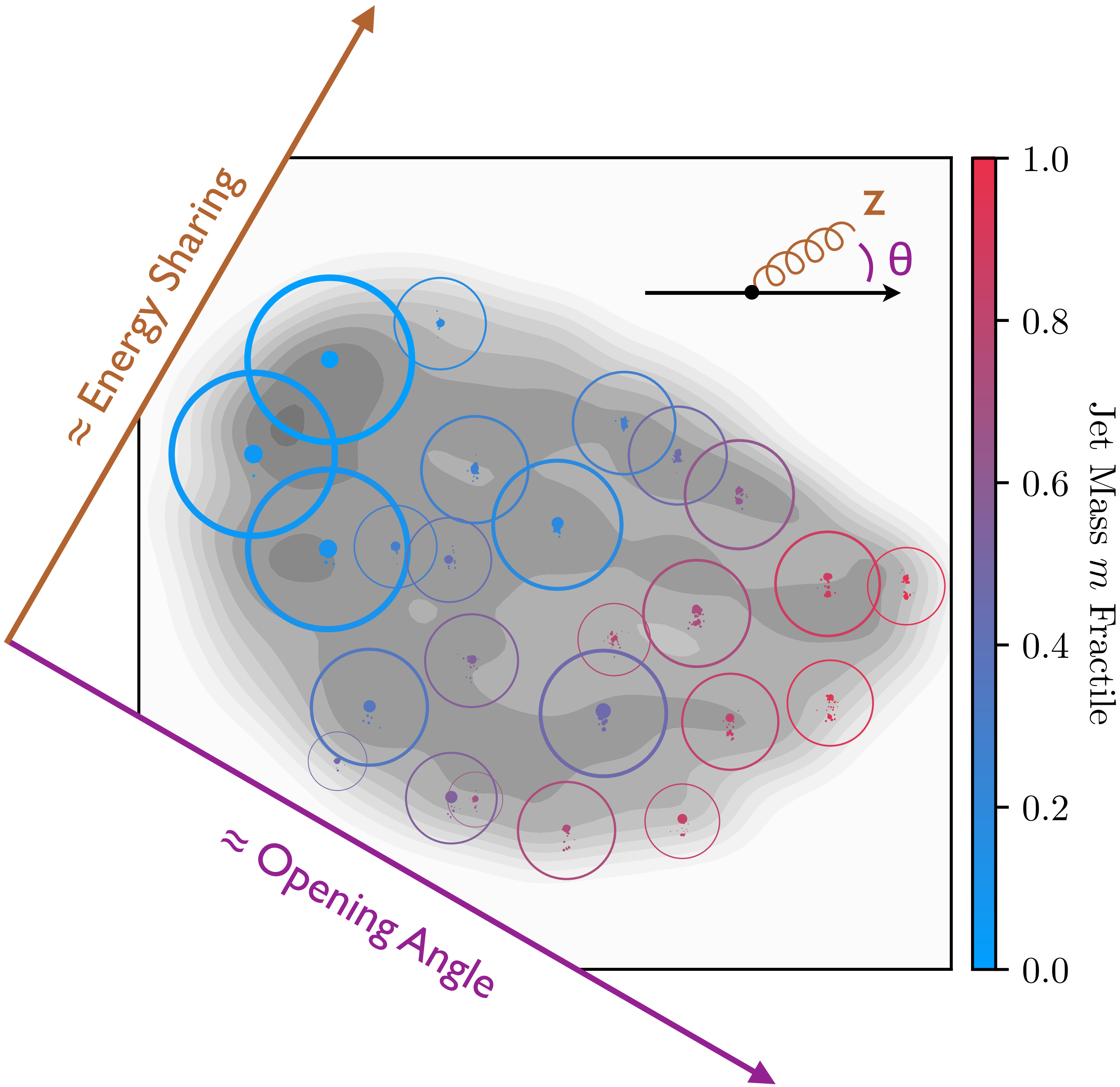


[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020]
[using van der Maaten, Hinton, JMLR 2008; using CMS Open Data]



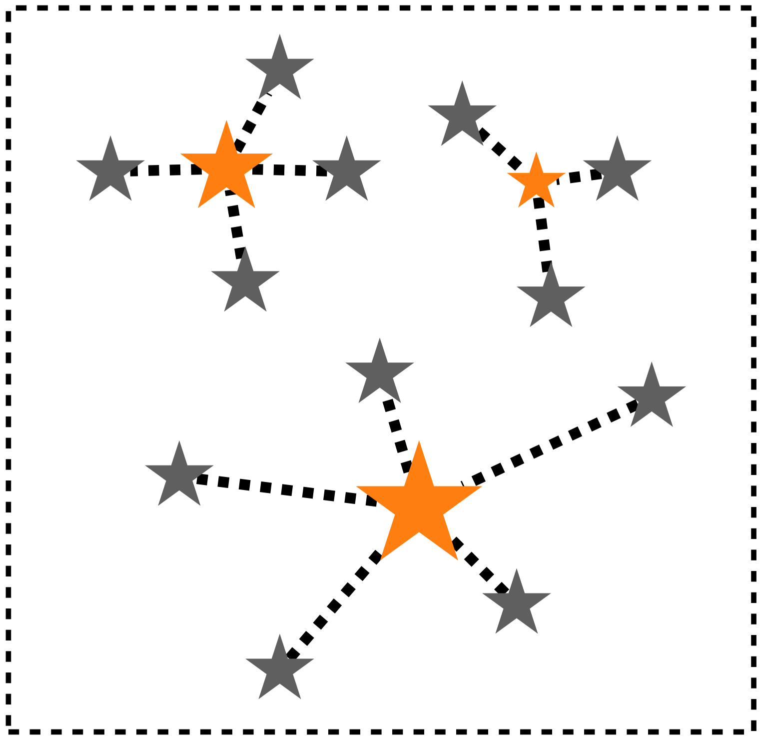
Most Representative Jets

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



k-medoids

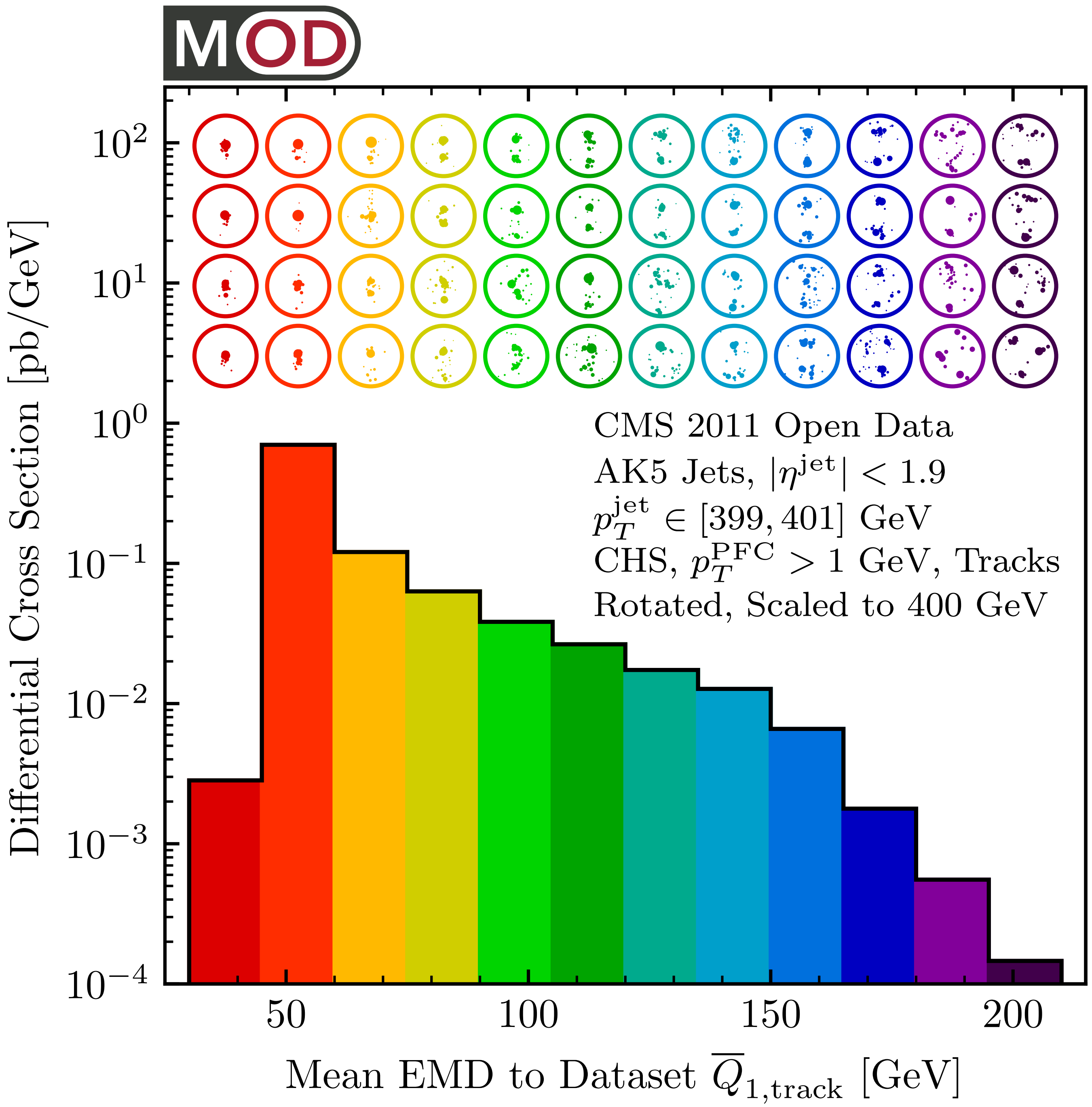
Arranged via t-SNE



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

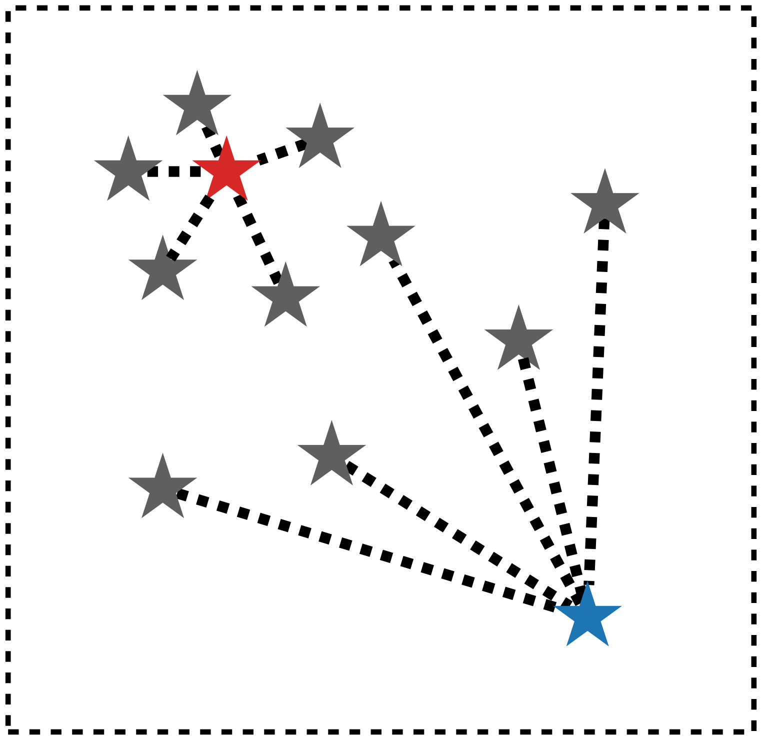
Least Representative Jets

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



New Physics?

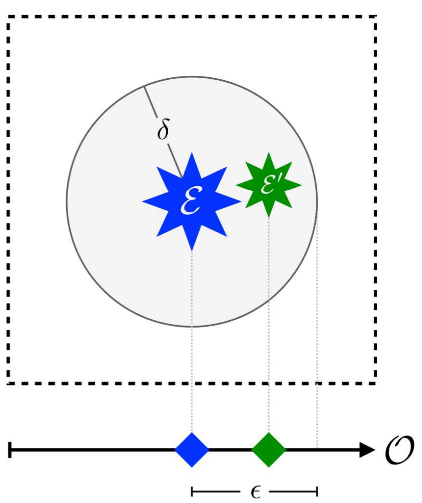
Or tails of QCD?



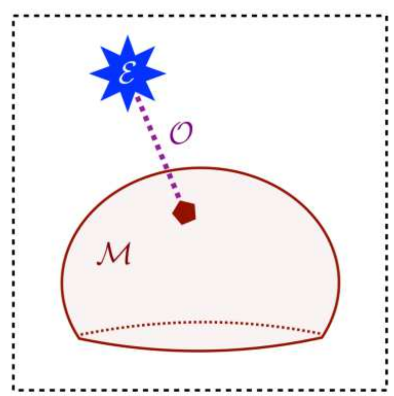
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020]
[using CMS Open Data]

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

IRC Safety is smoothness in the space of events

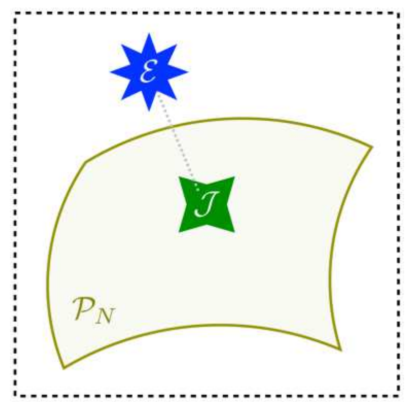


Event shapes are distances from events to manifolds.



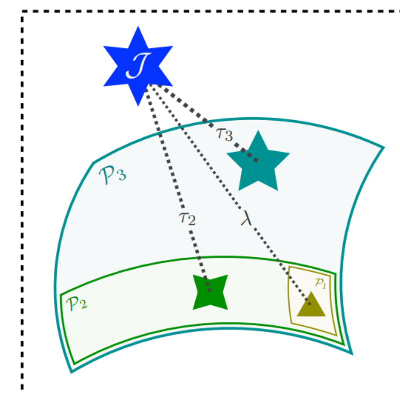
$\mathcal{O}(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{M}} \text{EMD}_{\beta,R}(\mathcal{E}, \mathcal{E}')$

Jets are projections to few-particle manifolds.



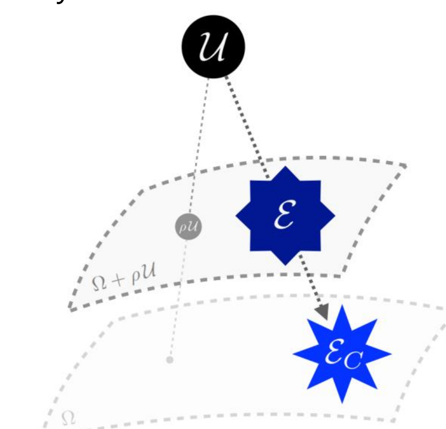
$\mathcal{J} = \underset{\mathcal{E}' \in \mathcal{P}_N}{\text{argmin}}\, \text{EMD}_{\beta,R}(\mathcal{E}, \mathcal{E}')$

Substructure resolves emissions within the jet.



$\tau(\mathcal{J}) = \min_{\mathcal{E}' \in \mathcal{P}_N} \text{EMD}_{\beta}(\mathcal{J}, \mathcal{E}').$

Pileup mitigation moves away from uniform radiation.



$\mathcal{E}_C = \arg\min_{\mathcal{E}'} \text{EMD}(\mathcal{E}, \mathcal{E}' + \rho\, \mathcal{U})\,.$

Taming infinities — Event Shapes — Jet Algorithms — Jet Substructure — Pileup

1960 — 2020

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

1977
Thrust, Sphericity
[Farhi, PRL 1977]
[Georgi, Machacek, PRL 1977]

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

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

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

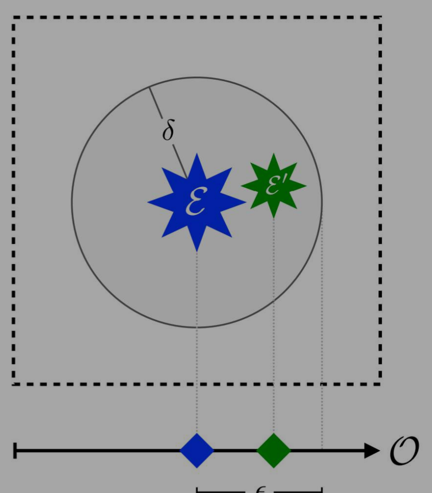
2014-2019
Constituent Subtraction
[Berta, Spousta, Miller, Leitner, JHEP 2014]
[Berta, Masetti, Miller, Spousta, JHEP 2019]

And many more!

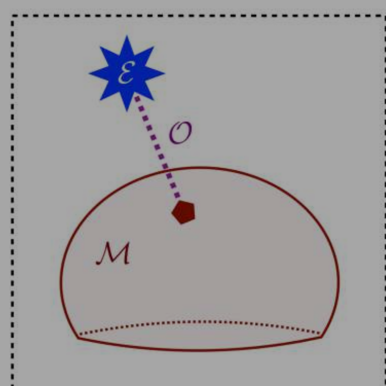
[timeline from Eric Metodiev; Komiske, Metodiev, JDT, JHEP 2020]

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

IRC Safety is smoothness in the space of events

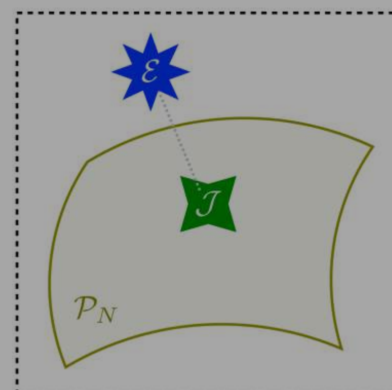


Event shapes are distances from events to manifolds.



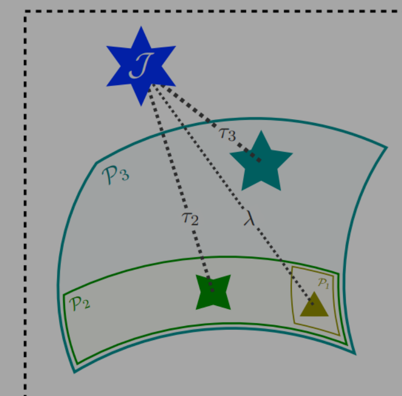
$\mathcal{O}(\mathcal{E}) = \min_{\mathcal{E}'\in\mathcal{M}} \mathrm{EMD}_{\beta,R}(\mathcal{E},\mathcal{E}')$

Jets are projections to few-particle manifolds.



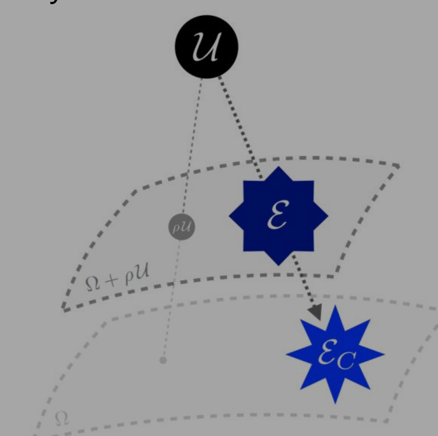
$\mathcal{J} = \operatorname{argmin}_{\mathcal{E}'\in\mathcal{P}_N} \mathrm{EMD}_{\beta,R}(\mathcal{E},\mathcal{E}')$

Substructure resolves emissions within the jet.



$\tau(\mathcal{J}) = \min_{\mathcal{E}'\in\mathcal{P}_N} \mathrm{EMD}_{\beta}(\mathcal{J},\mathcal{E}').$

Pileup mitigation moves away from uniform radiation.



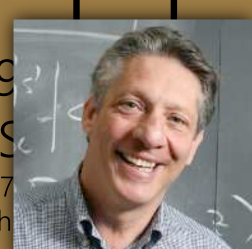
$\mathcal{E}_C = \arg\min_{\mathcal{E}'} \mathrm{EMD}(\mathcal{E},\mathcal{E}'+\rho\,\mathcal{U})\,.$

Taming infinities | Event Shapes | Jet Algorithms | Jet Substructure | Pileup

1960 — 2020

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

19
Thrust, S
[Farhi, PRL 197
[Georgi, Mach



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

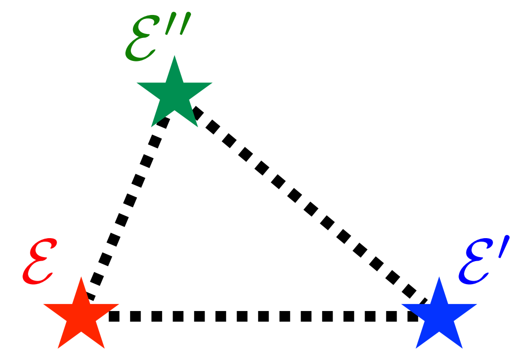
1997-1998
C/A jet clustering
[Wobisch, Wengler, 1998]
[Doskhitzer, Leder, Moretti,Webber, JHEP 1997]

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

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:

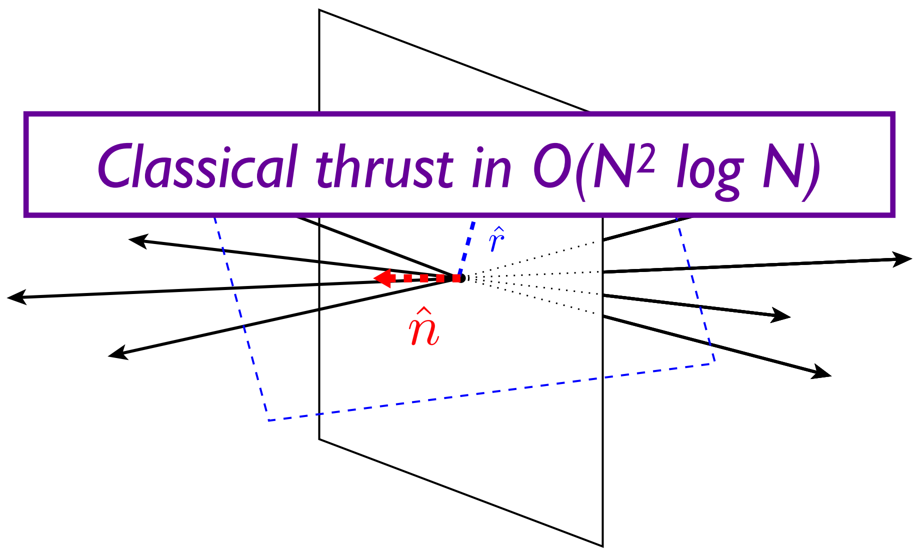
Potential polynomial improvements over classical algorithms

Classical Development:

New geometric data analysis strategy for collider physics

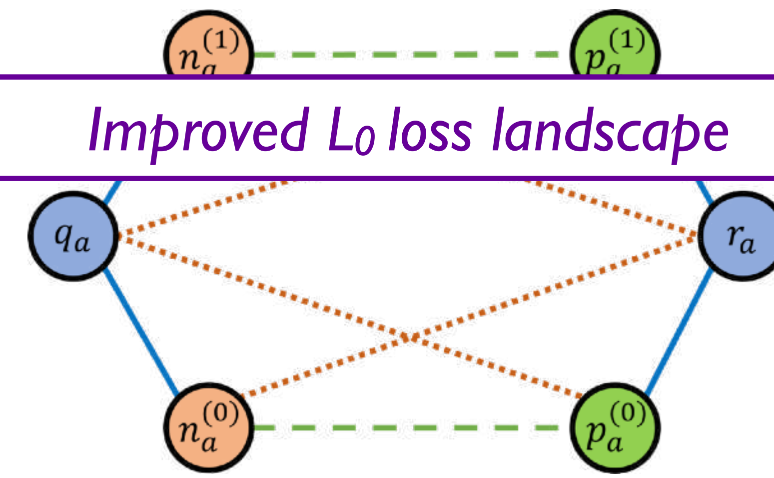
Quantum (Inspired) Algorithms for Colliders

Challenge of Data Loading



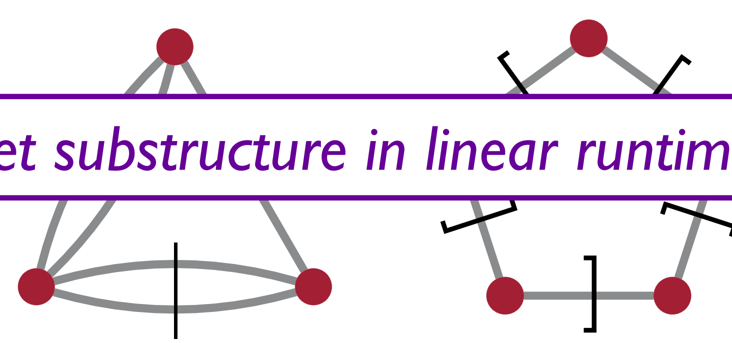
Classical thrust in O(N² log N)

Degeneracy Engineering



Improved L_0 loss landscape

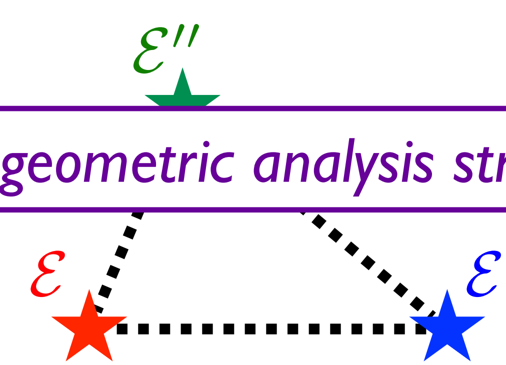
Superposition for Graphs



Jet substructure in linear runtime

Optimal Transport

if time permits



New geometric analysis strategies

Evangelizing one last time for QIS/HEP…

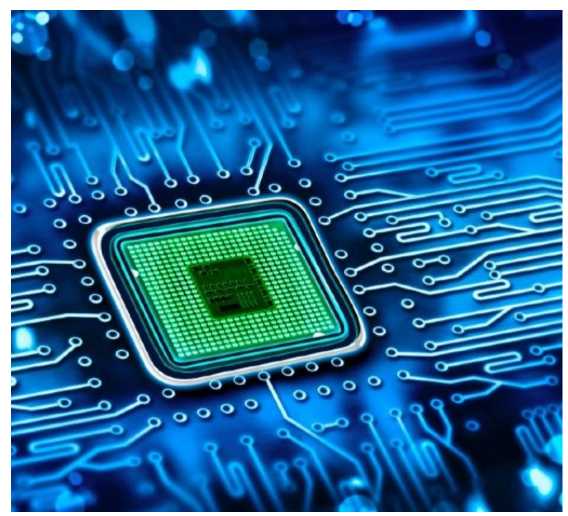
Slides from 2020 pandemic slide deck

Quantum Algorithms for HEP

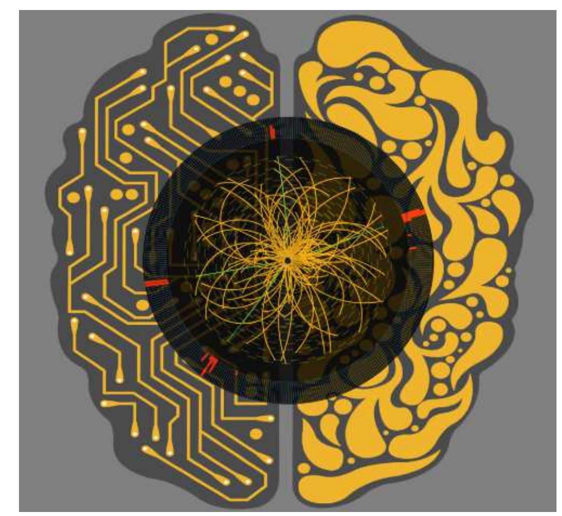
Simulation, Reconstruction & Analysis

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

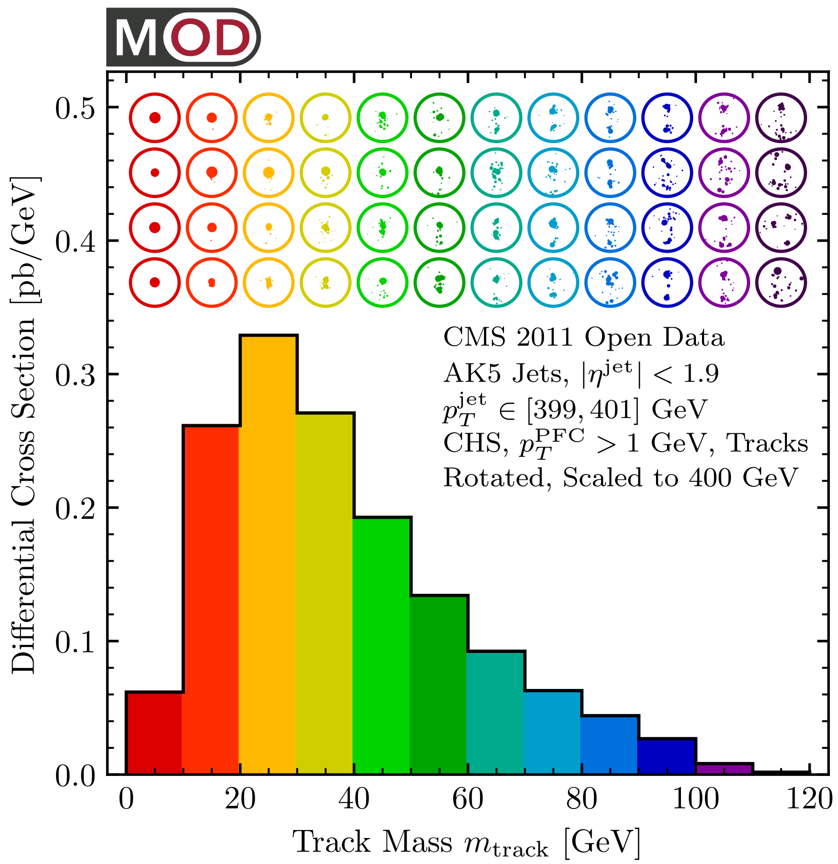
Collider Event

Every 25 nanoseconds at the LHC

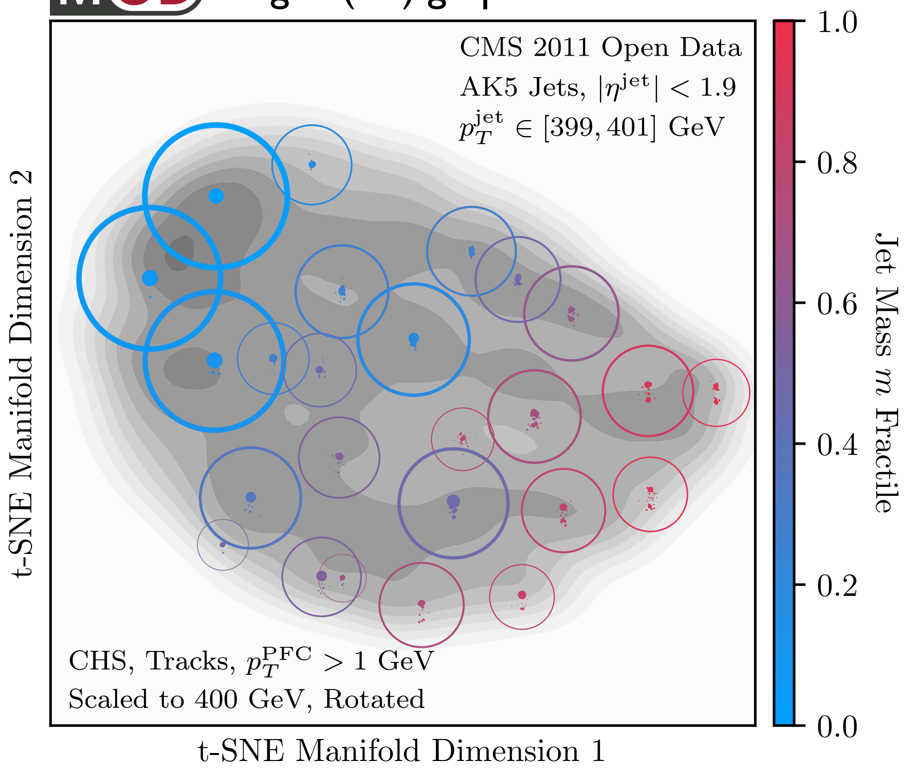
T E H M

γ photon

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



MOD e.g. O(N²) graph construction

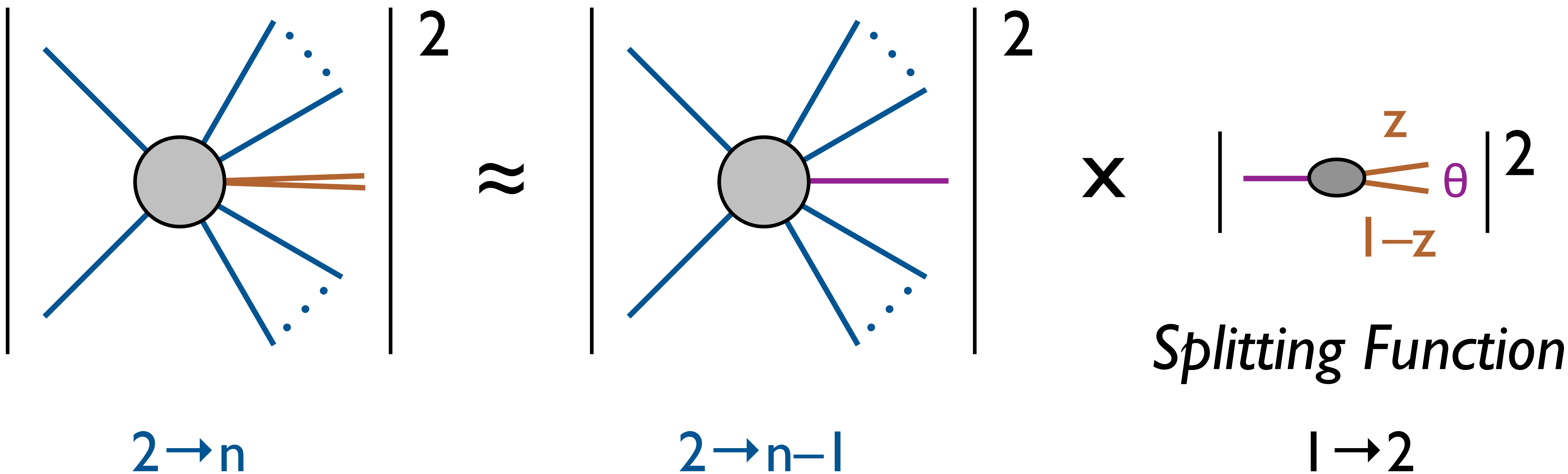


For quantum advantage, must start from harder classical problems

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

Factorization Suppresses Quantum Interference

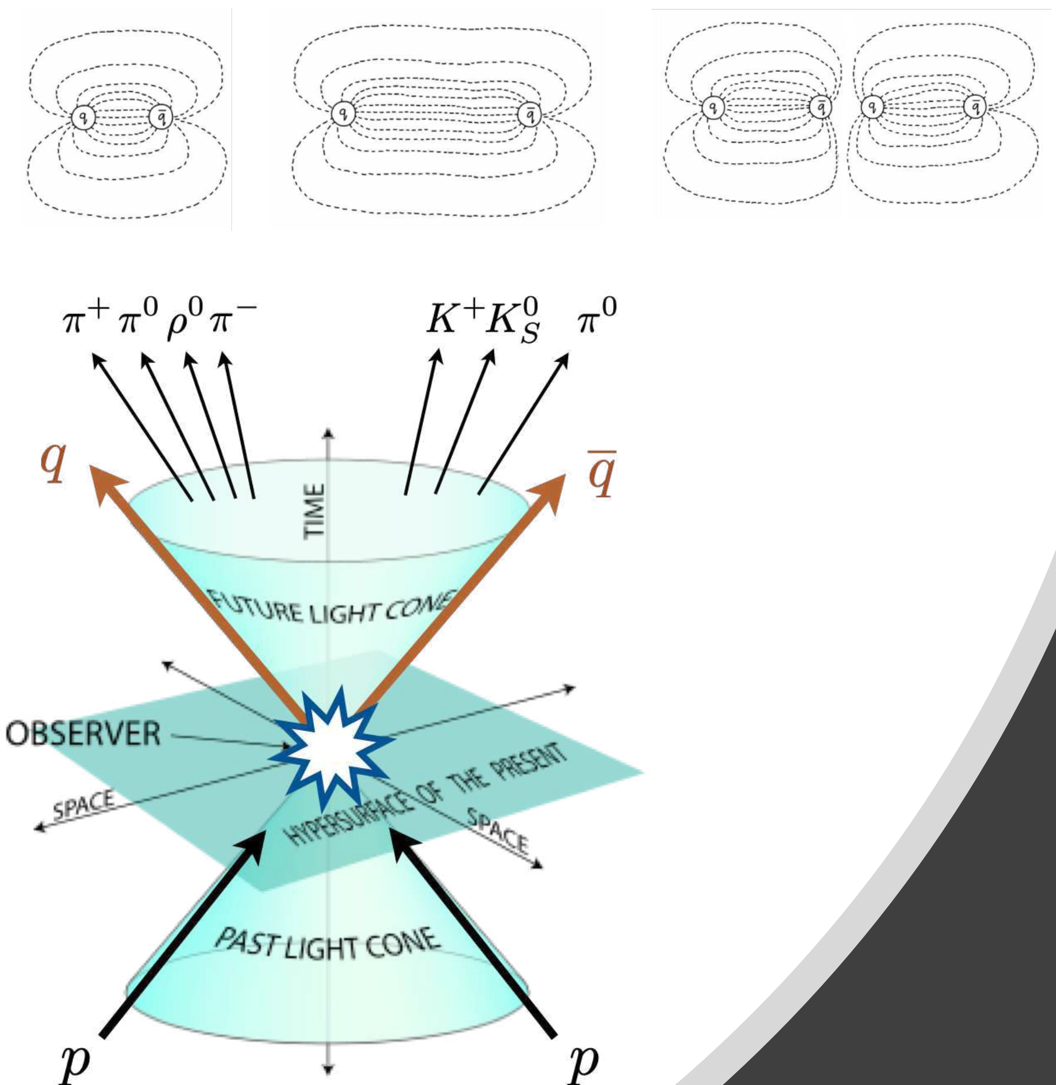
In soft/collinear limit of QCD, aspects of perturbative
quantum field theory becomes semi-classical



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



Real-time Dynamics of QCD Hadronization?

Light-like partons ⇒ time-like hadrons?

Parton distribution functions:
Prob. to find parton inside hadron

Jet fragmentation functions:
Prob. to find hadron from showering of parton

Excellent phenomenological models…
…but limited first principles understanding

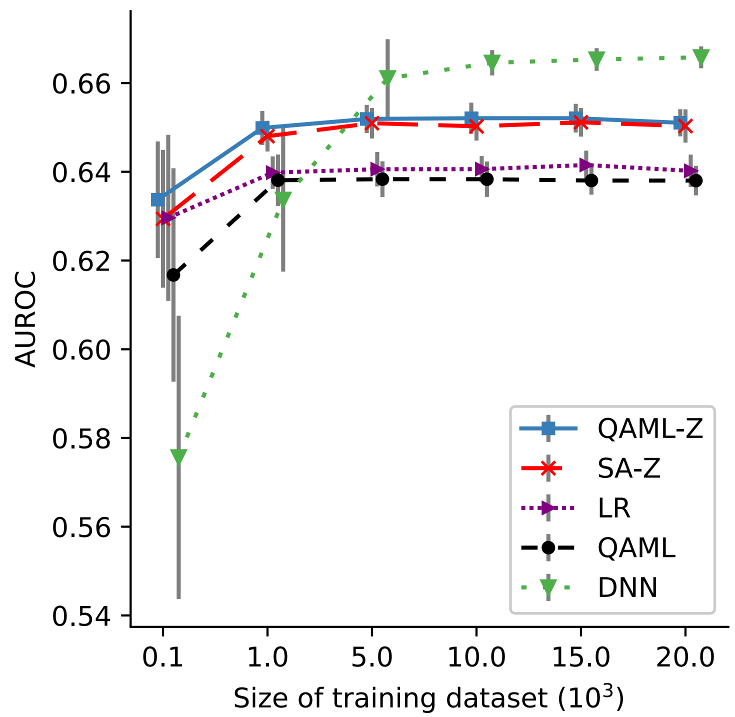
No rigorous quantum definition yet (to my knowledge)

Ultimately: extract from quantum simulation

[slide from C²QA meet & greet]

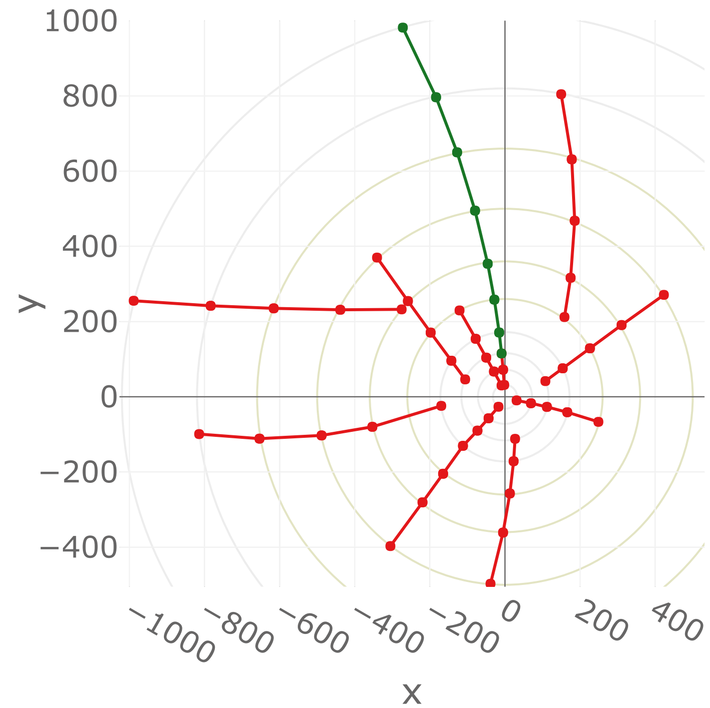
Quantum Algorithms for HEP

Simulation, Reconstruction & Analysis



Higgs Boson Identification

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



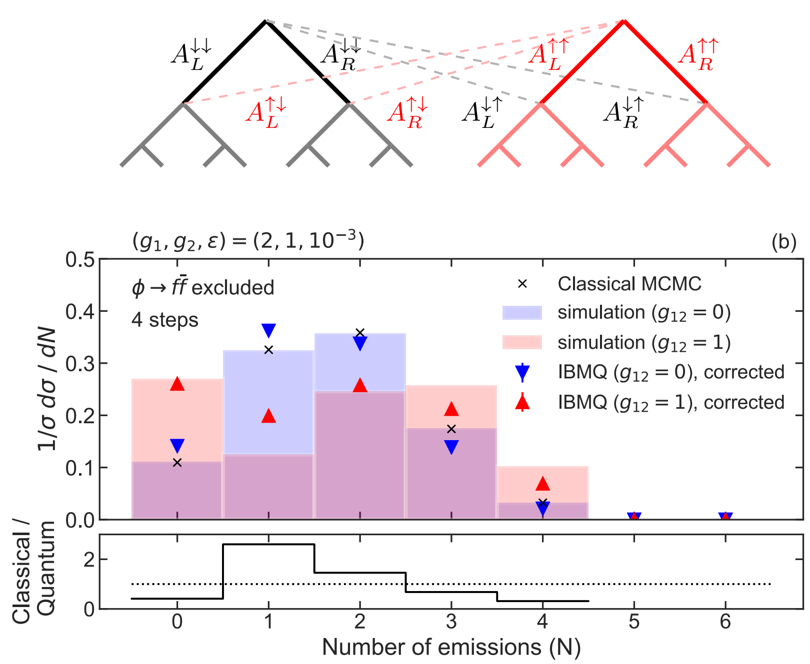
Track Reconstruction

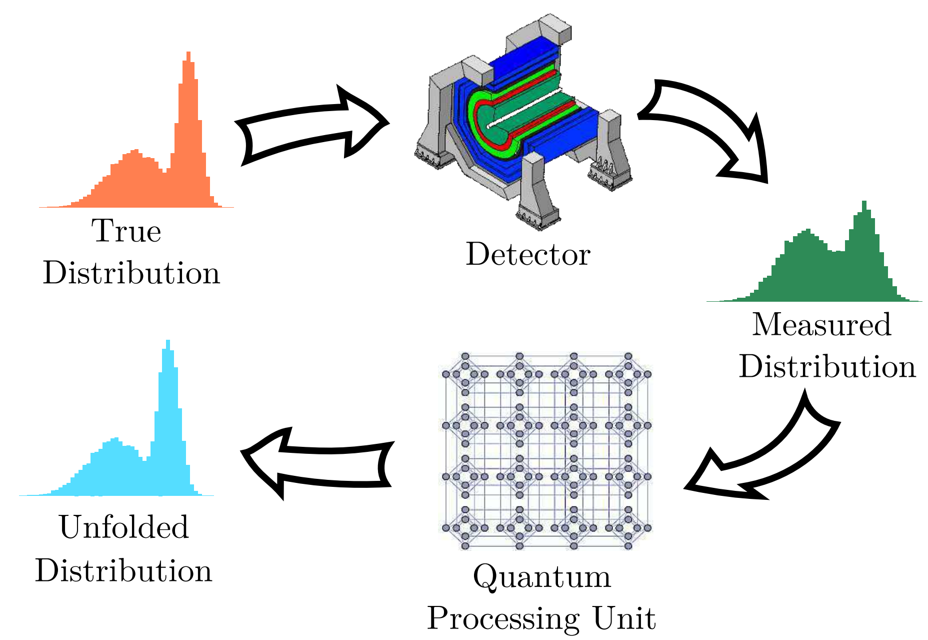
[Shapoval, Calafiura, CHEP 2018]
[Bapst, Bhimji, Calafiura, Gray, Lavrijsen, Linder, CSBS 2020]
[Zlokapa, Anand, Vlimant, Duarte, Job, Lidar, Spiropulu, arXiv 2019]

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

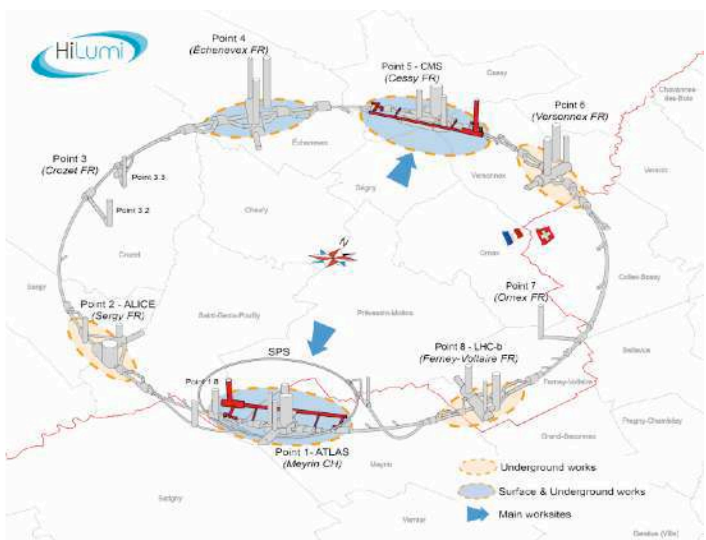
Collider Event

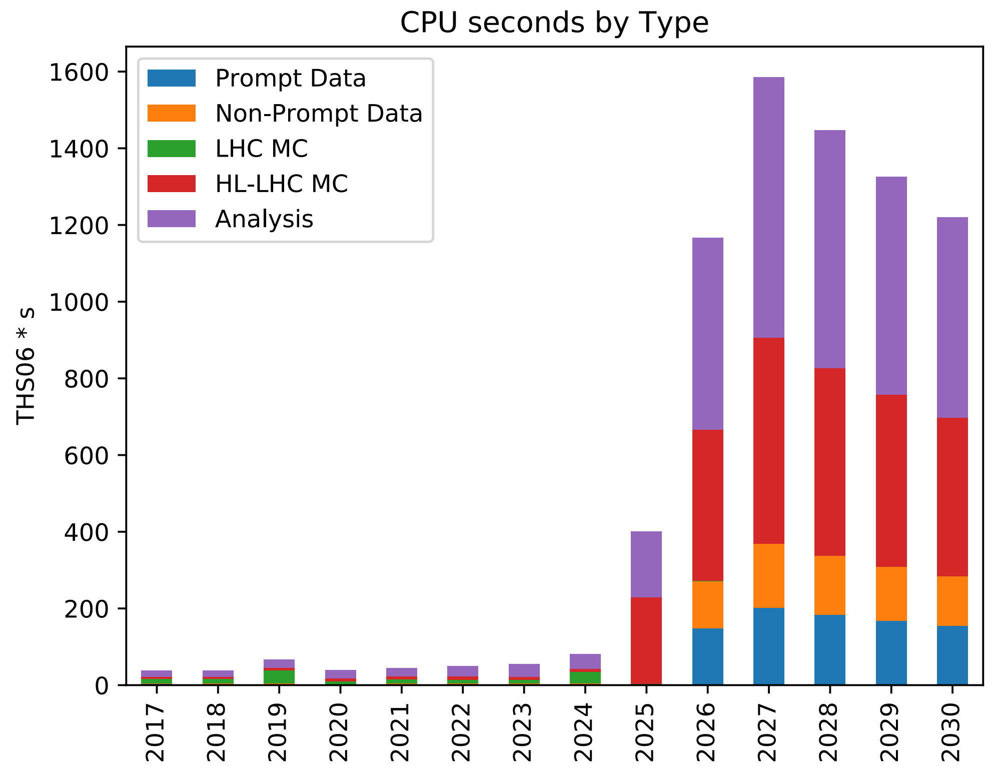
Every 25 nanoseconds at the LHC

T E H M

γ photon

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





Analysis

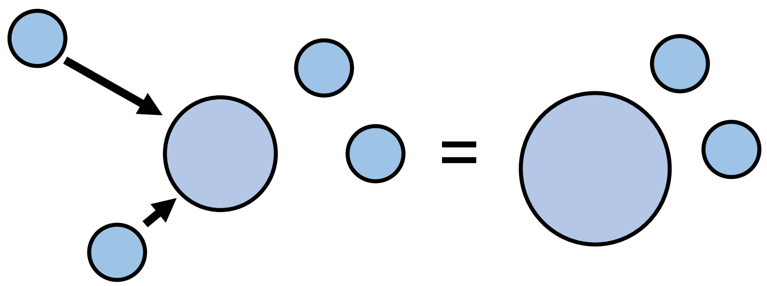
Simulation

Reconstruction

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



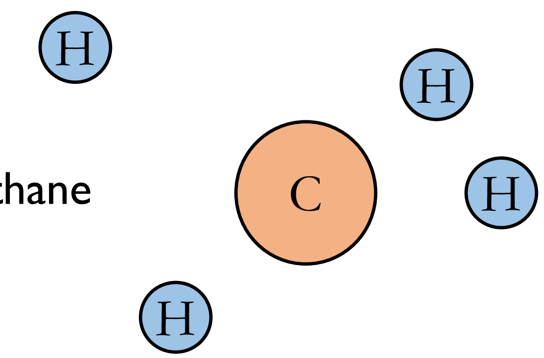
Molecular Symmetries and Quantum Field Theory?

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

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

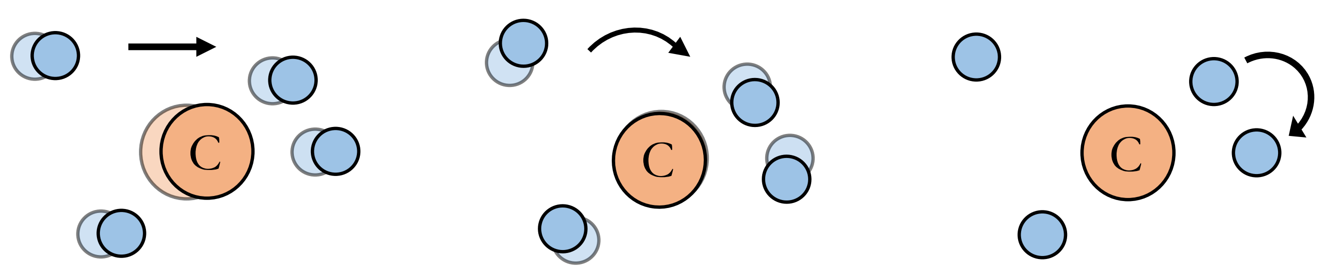
nuclear charges   nuclear positions

e.g. methane



What are the symmetries of E?

translation   rotation   permutation



Are there hidden symmetries?

Focus on Electronic Energy

Known Analytically!

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

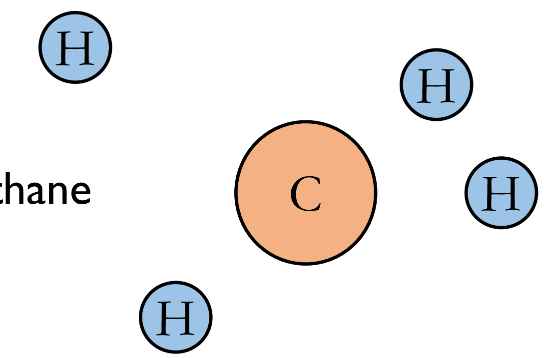
Molecular Symmetries and Quantum Field Theory?

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

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

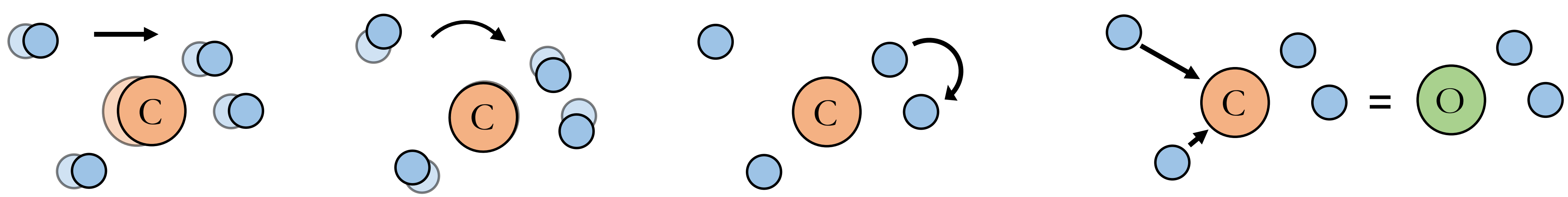
nuclear charges nuclear positions

e.g. methane



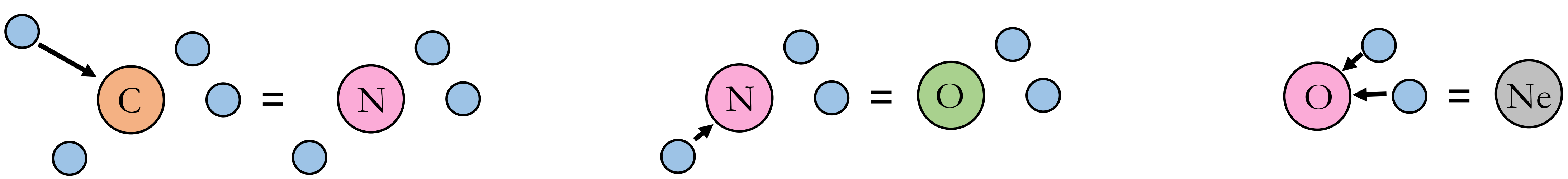
What are the symmetries of $E_{\mathbf{elec}}$?

translation rotation permutation **united atom**



United Atom Symmetry is extremely constraining!

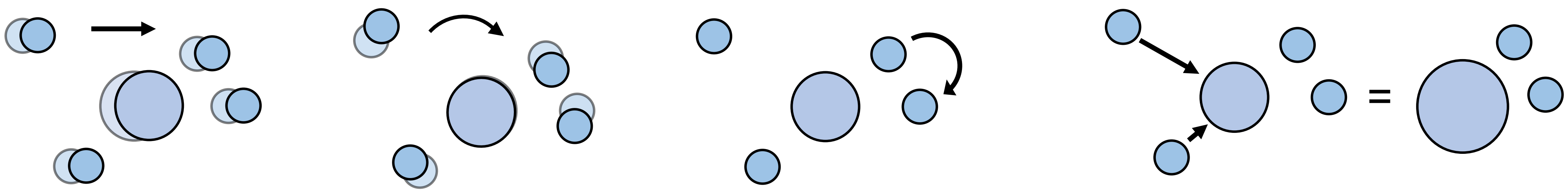
E.g.: knowing configuration energies of **methane** specifies properties of **ammonia** and **water**.



Molecular Symmetries and Quantum Field Theory?

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

boost | rotation | permutation | **infrared and collinear safety**



Mathematically identical to the molecular symmetries!

Scattering Symmetries		**Molecular Symmetries**
Particle Energy E_i	$\longleftrightarrow$	Nuclear Charge Z_i
Particle Direction $\hat{n}_i$	$\longleftrightarrow$	Nuclear Position $\vec{r}_i$

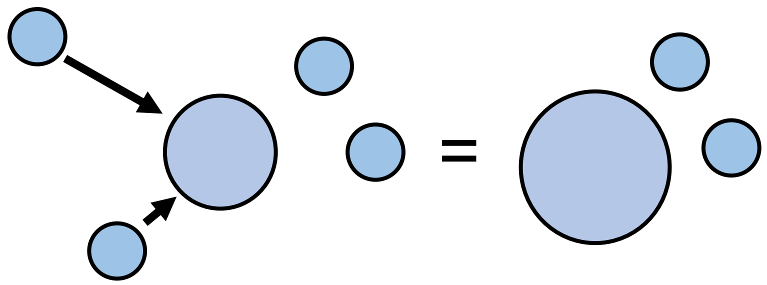
Ongoing work: We can directly apply our developments from collider physics.

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

Polynomial basis with full symmetries
[Komiske, Metodiev, Thaler 1712.07124]

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

Symmetric machine learning architecture for molecules
[Komiske, Metodiev, Thaler 1810.05165]



Quantum Inspiration:

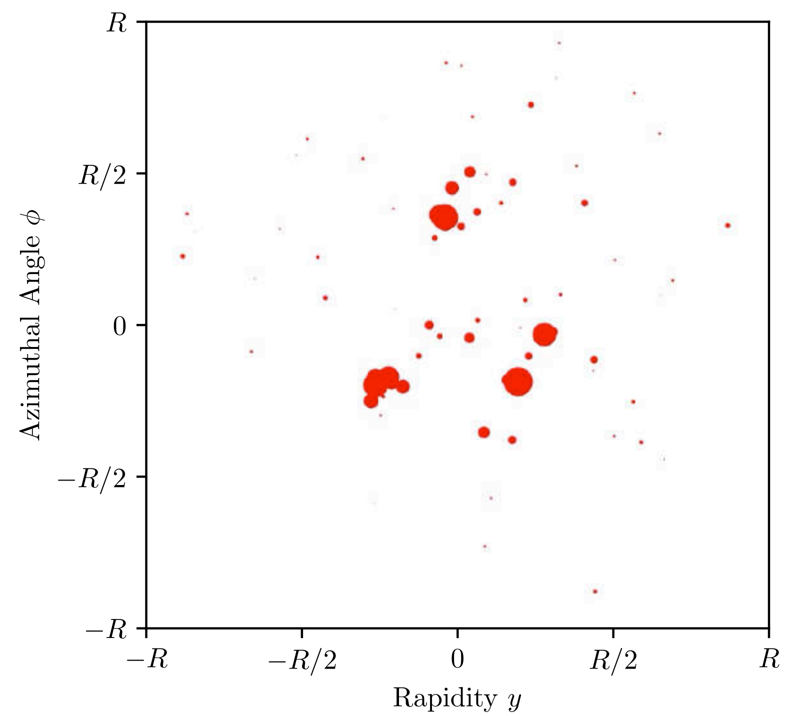
Encoding symmetries of electron wave functions

Classical Development:

Map between IRC safety (QFT) and united atom (chemistry)

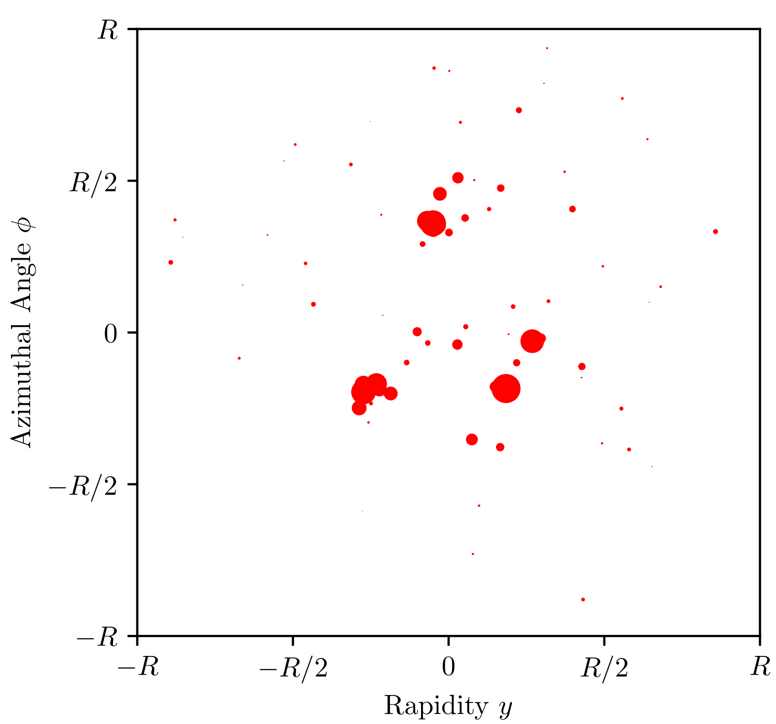
Similarity of Two Energy Flows?

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

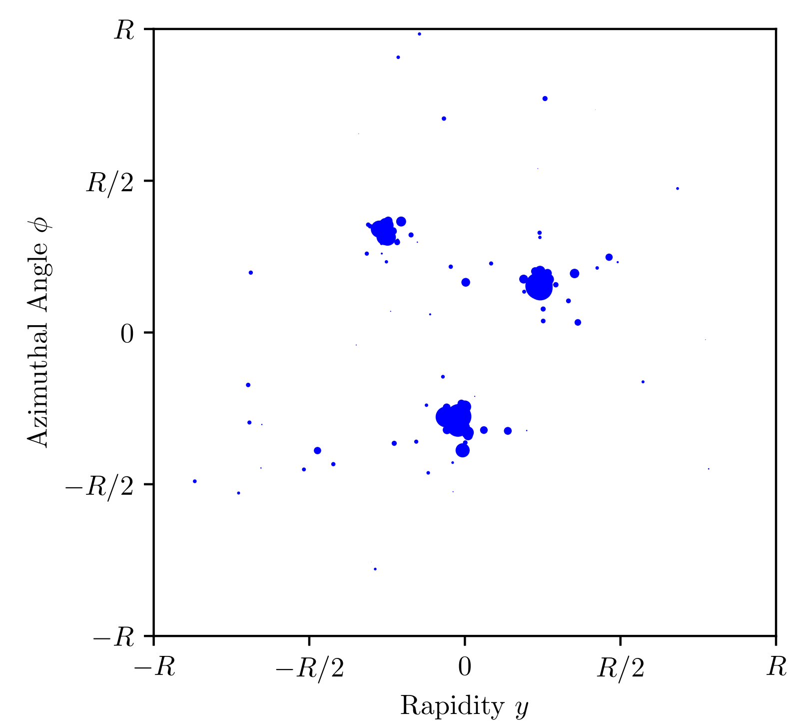


Optimal Transport:

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



125.4 GeV



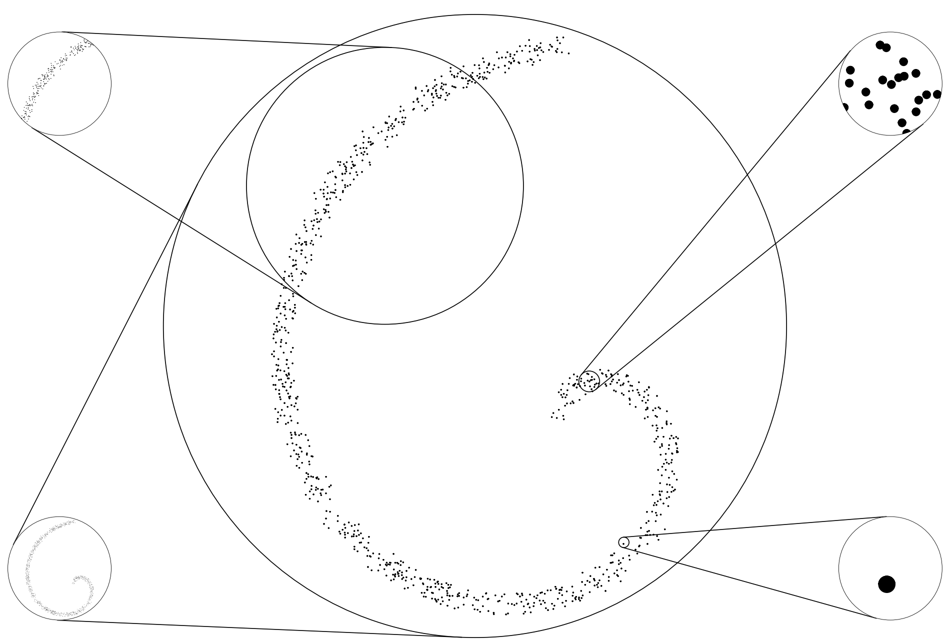
[Komiske, Metodiev, JDT, PRL 2019; code at Komiske, Metodiev, JDT, energyflow.network]

Dimensionality of Space of Jets

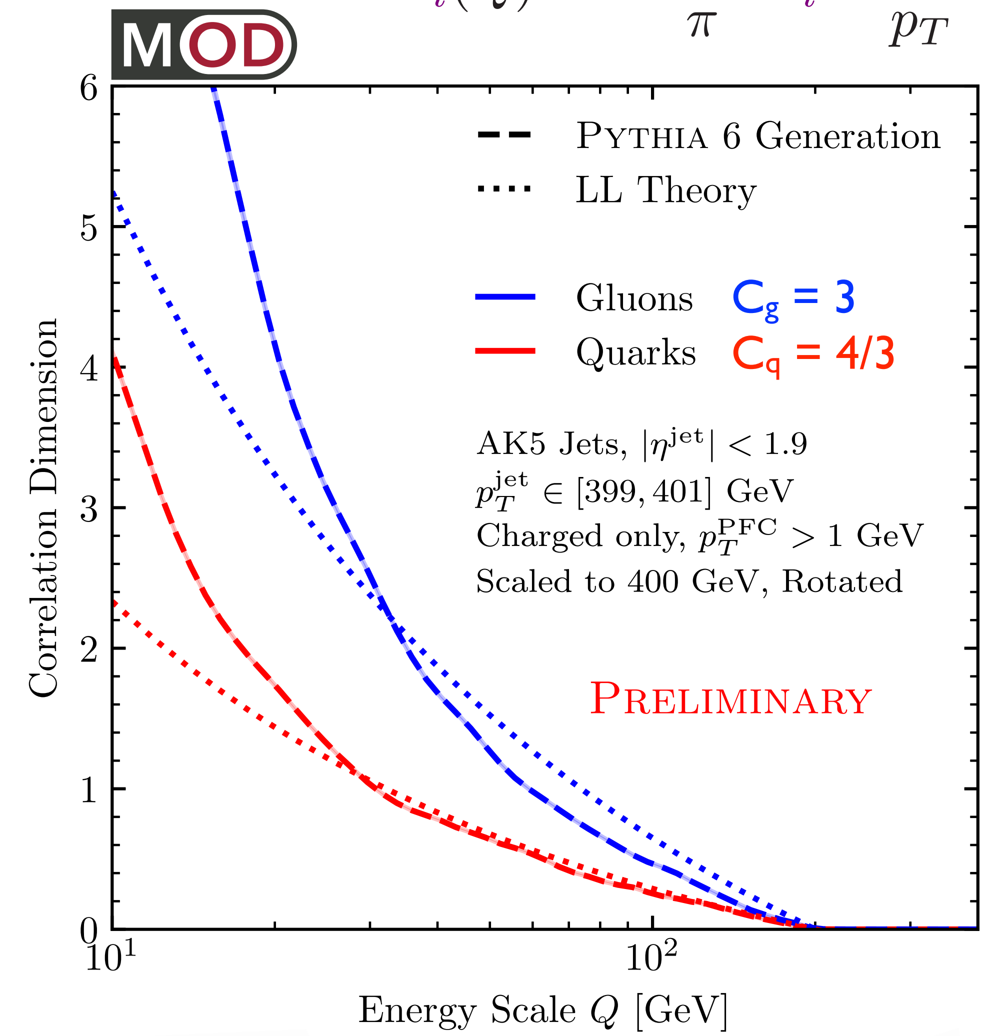
$$N_{\text{neighbors}}(r) \sim r^{\text{dim}}$$

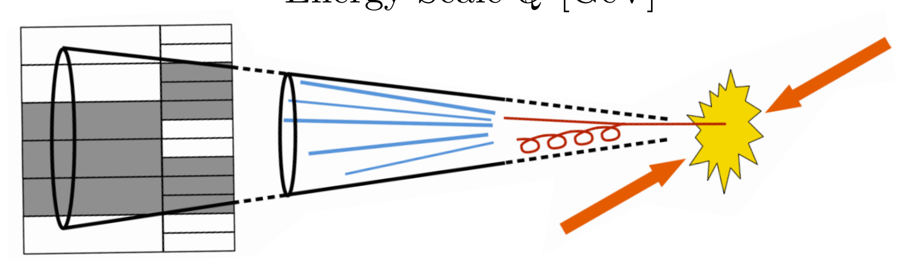
$$\Rightarrow \quad \text{dim}(r) \sim r \frac{\partial}{\partial r} \ln N_{\text{neighbors}}(r)$$

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



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





Dimensionality of Space of Jets

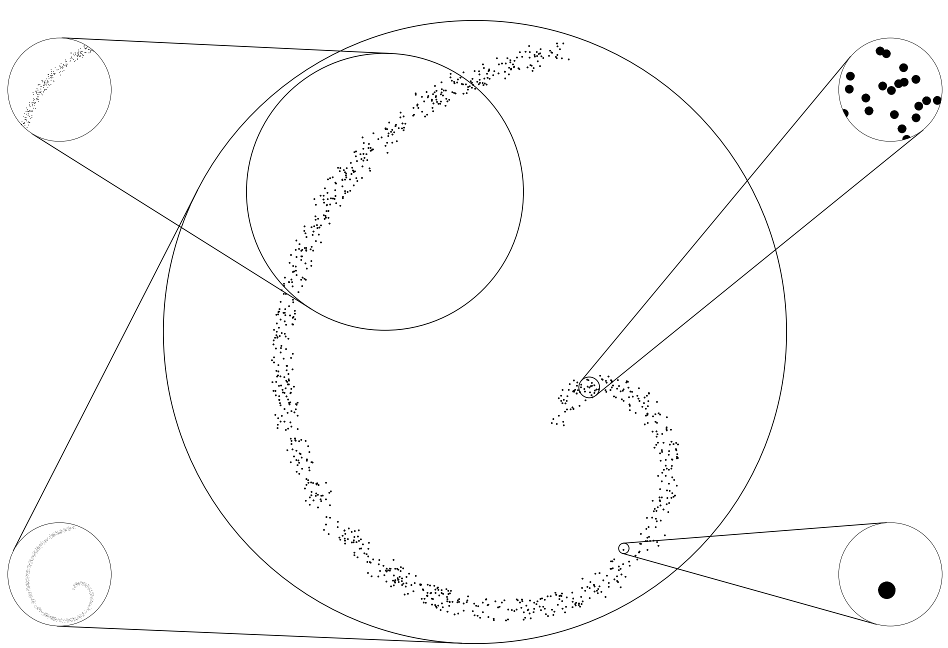
$$N_{\text{neighbors}}(r) \sim r^{\text{dim}}$$

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

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

dim≃1

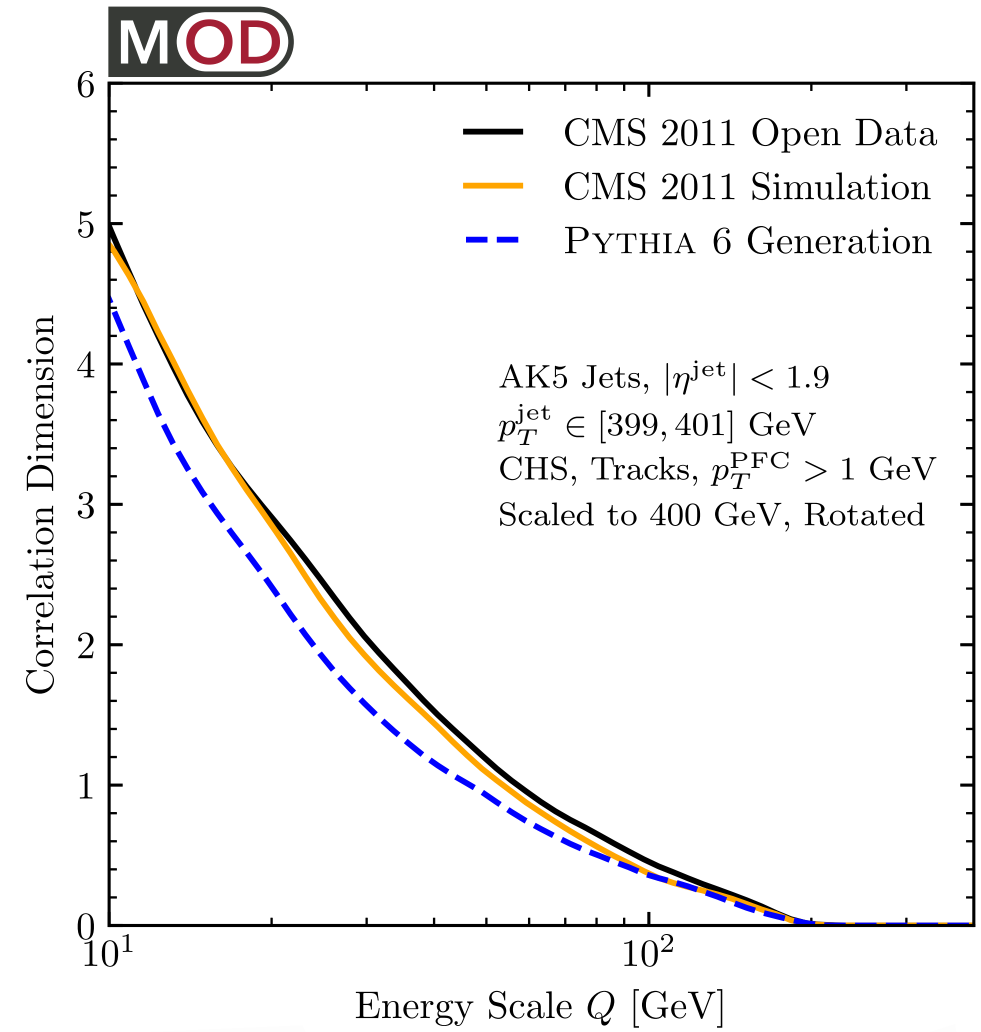
dim≃2

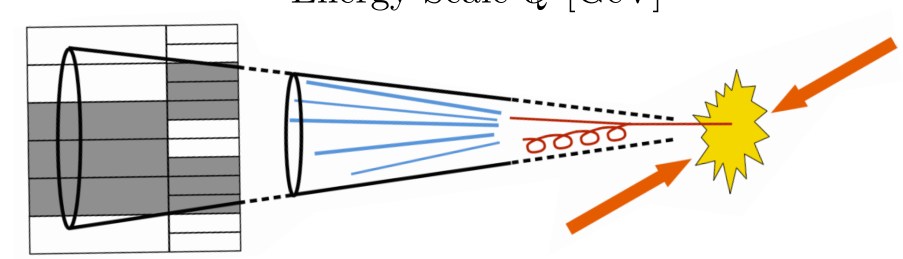


dim≃2

(eventually 0)

dim≃0

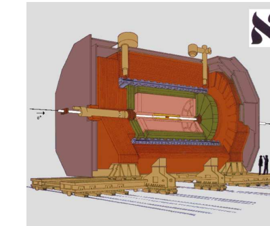




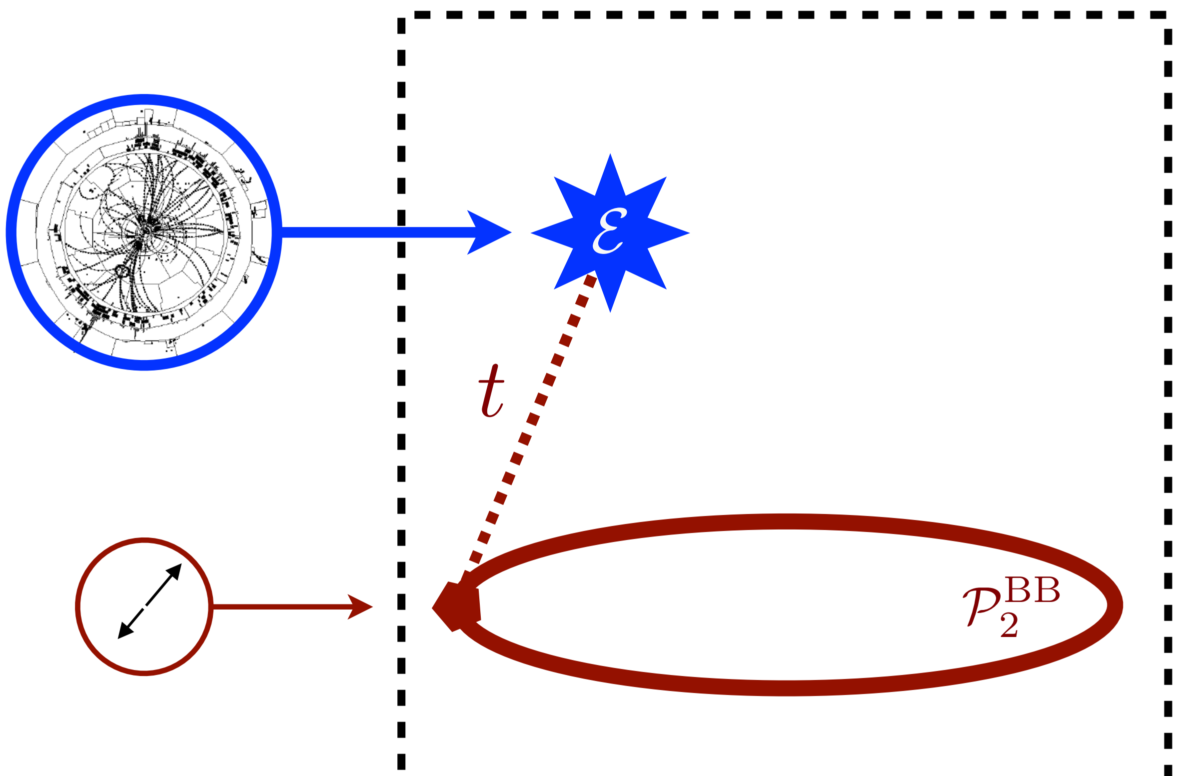
[Komiske, Mastandrea, Metodiev, Naik, JDT, PRD 2020;
using CMS Open Data]

E.g. Thrust

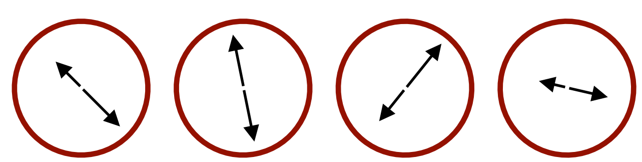
How dijet-like is an event?



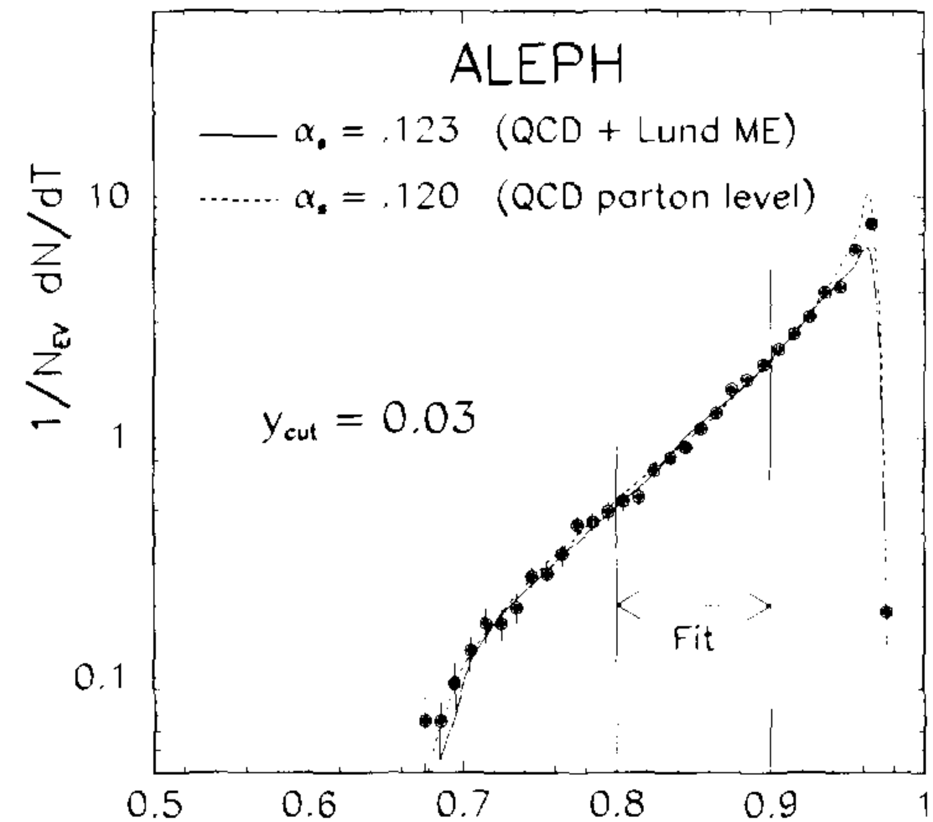
$$t(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{P}_2^{\rm BB}} \mathrm{EMD}_2(\mathcal{E}, \mathcal{E}')$$



All Back-to-Back Two Particle Configurations

$\mathcal{P}_2^{\rm BB} = \{$  $\cdots \}$

(using β=2 EMD variant)



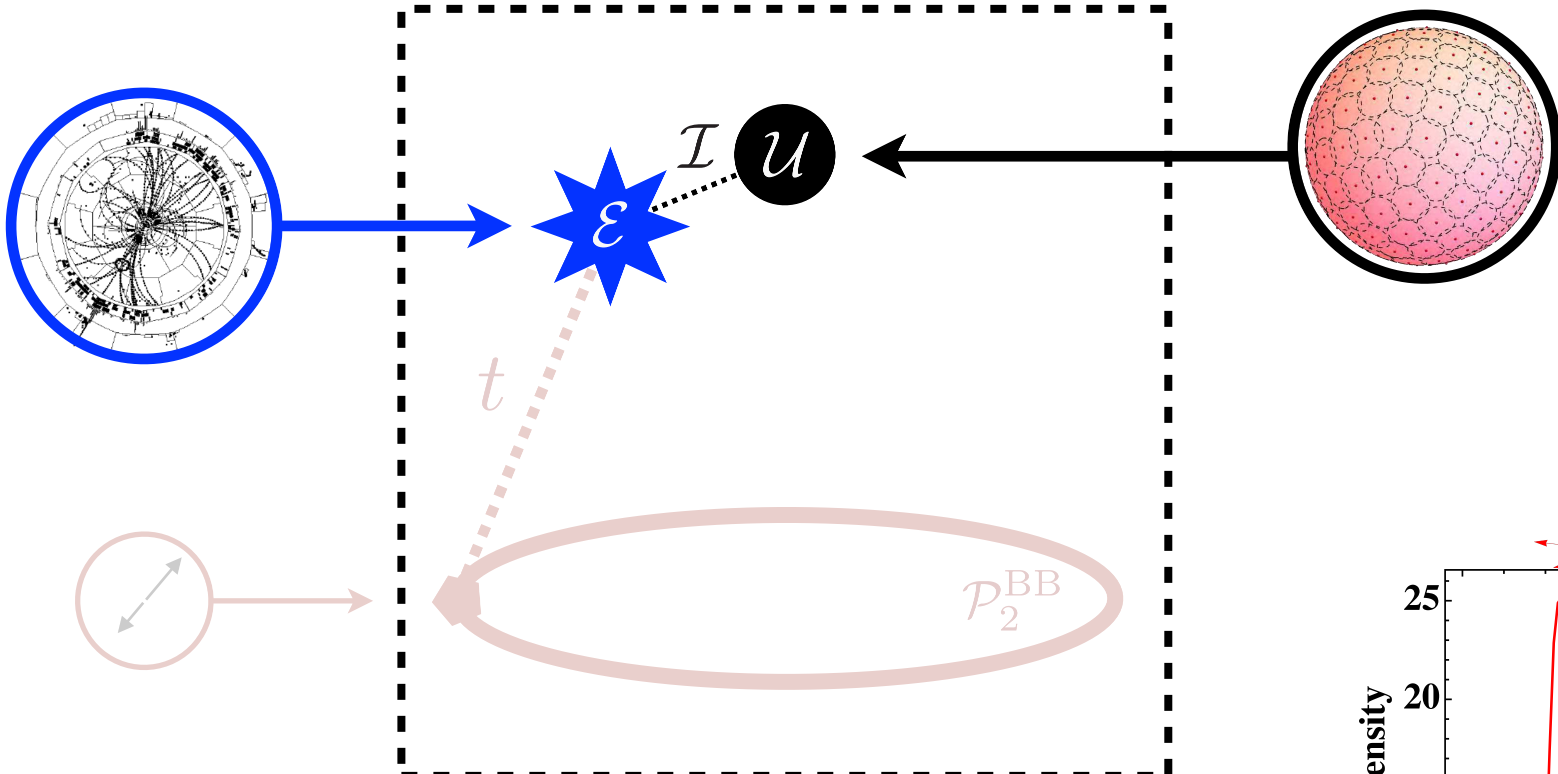
$$1 - \frac{t}{2E_{\rm CM}}$$

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

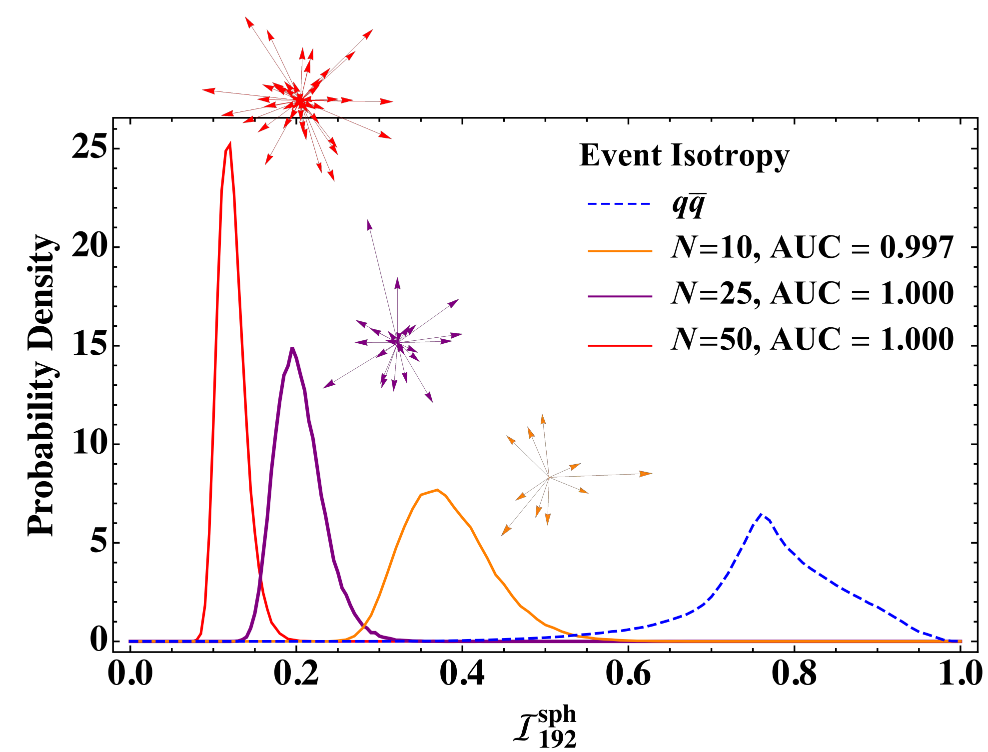
[Komiske, Metodiev, JDT, JHEP 2020]
[Brandt, Peyrou, Sosnowski, Wroblewski, PL 1964; Farhi, PRL 1977; ALEPH, PLB 1991]

New! Event Isotropy

How isotropic is an event?



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

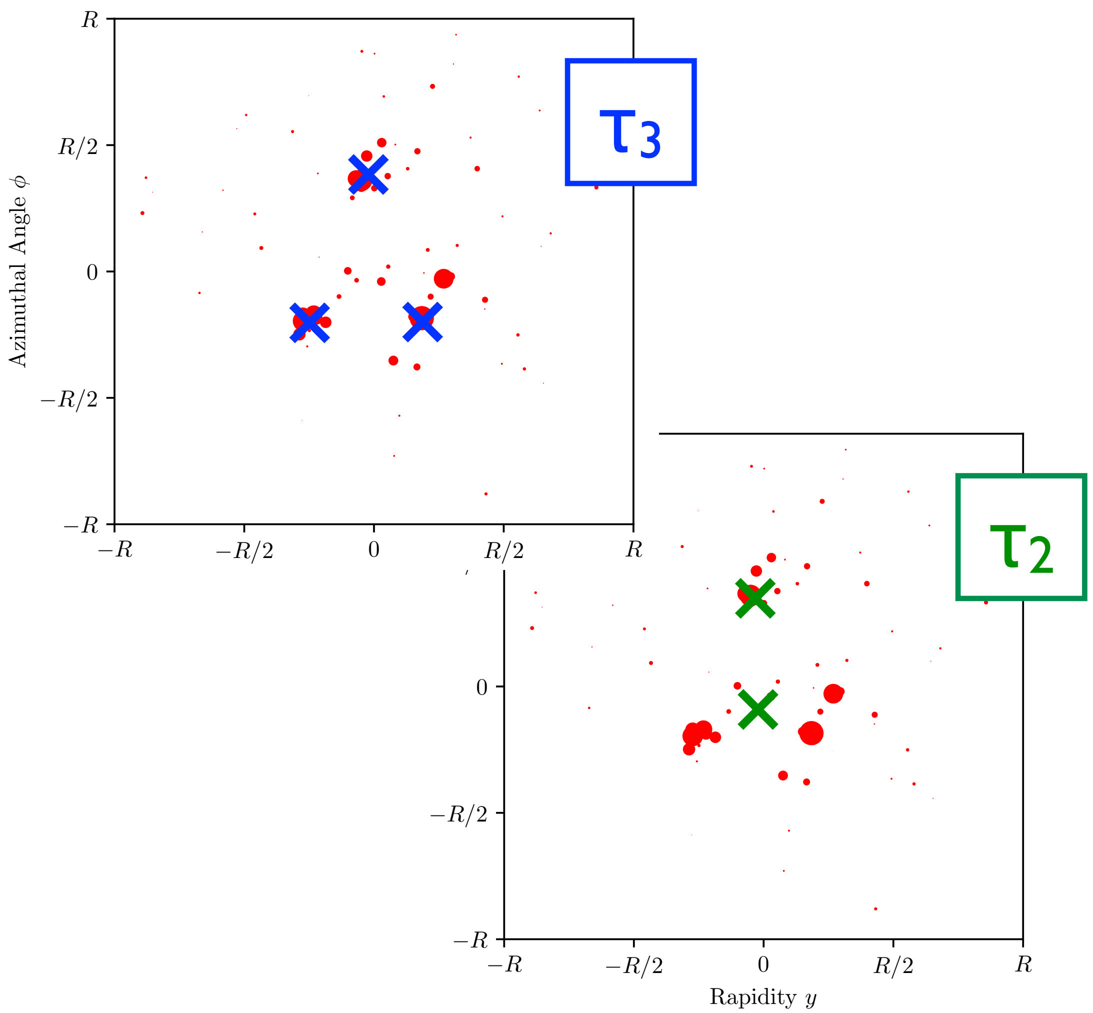


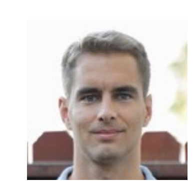
[Cesarotti, JDT, JHEP 2020;
see also Cesarotti, Reece, Strassler, JHEP 2021]

N-subjettiness

Ubiquitous jet substructure observable used for almost a decade…

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



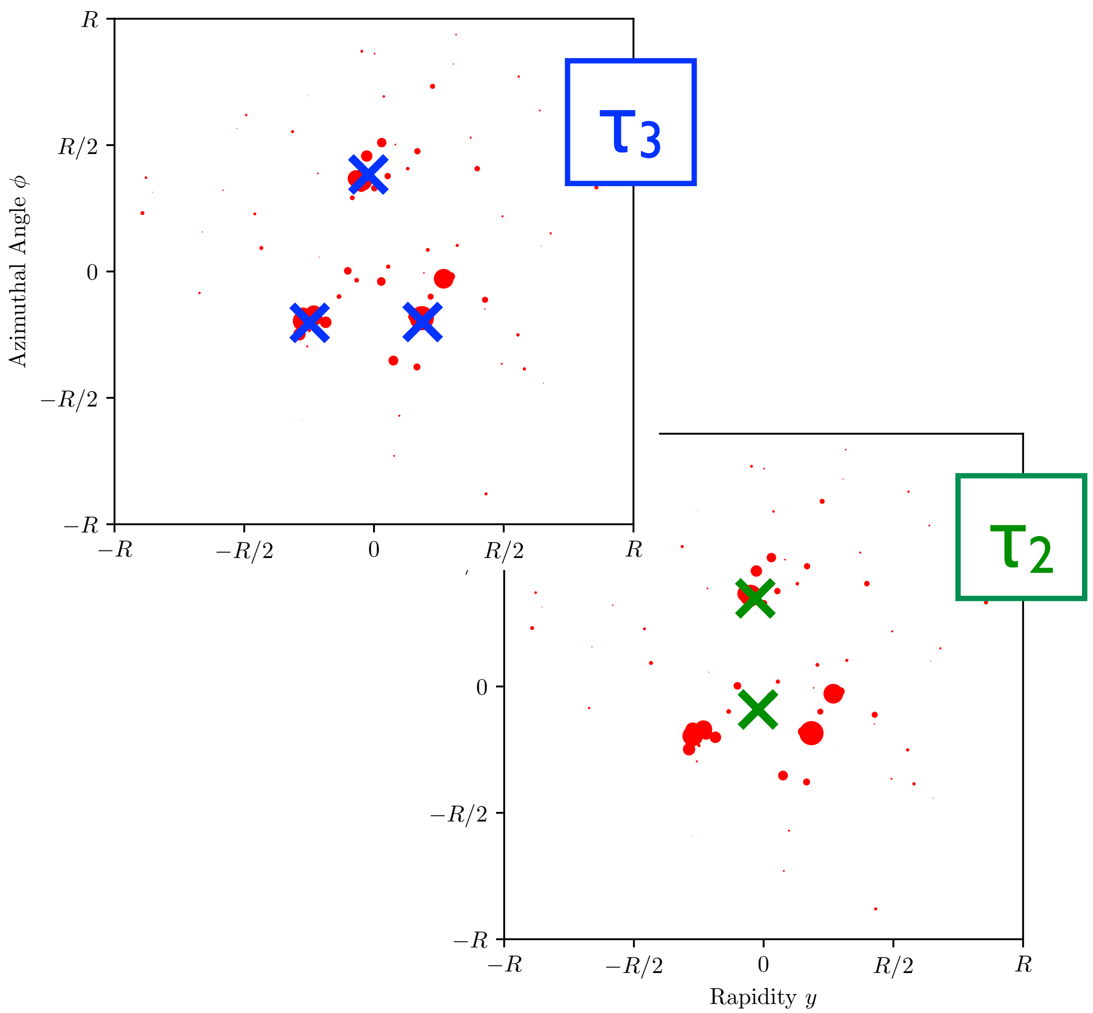


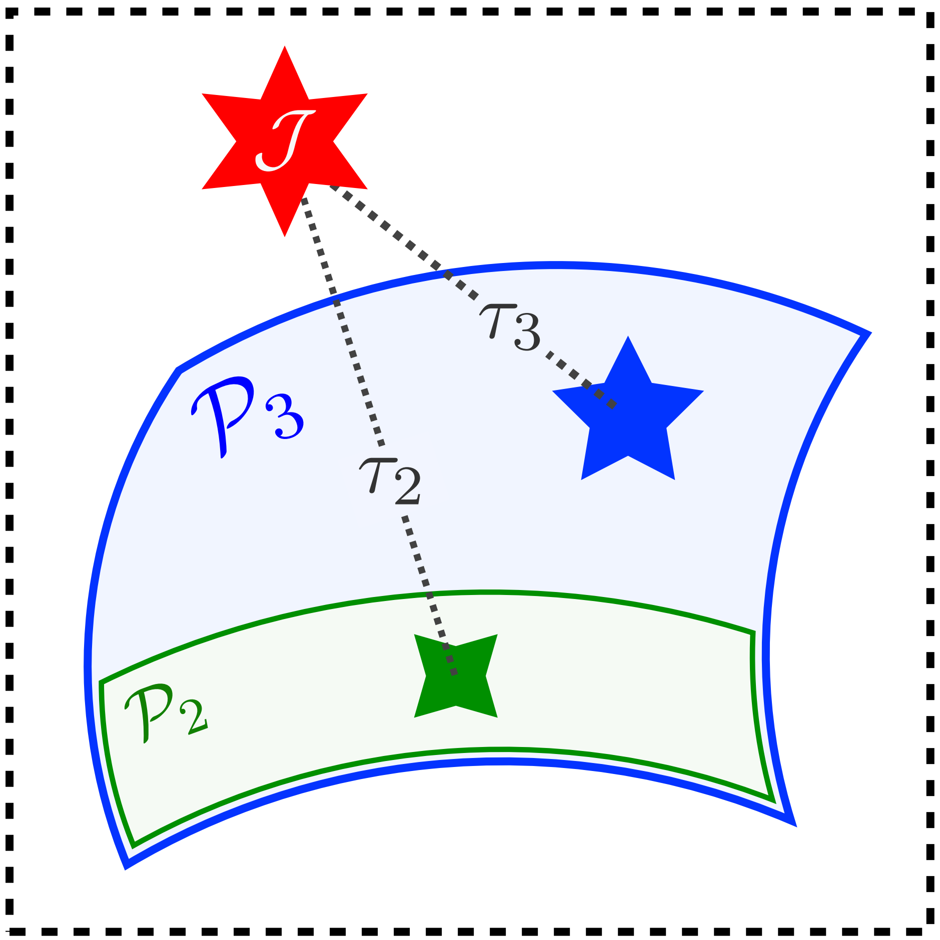
[JDT, Van Tilburg, JHEP 2011, JHEP 2012;
based on Brandt, Dahmen, ZPC 1979; Stewart, Tackmann, Waalewijn, PRL 2010]

N-subjettiness = Point to Manifold EMD

…is secretly an optimal transport problem

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



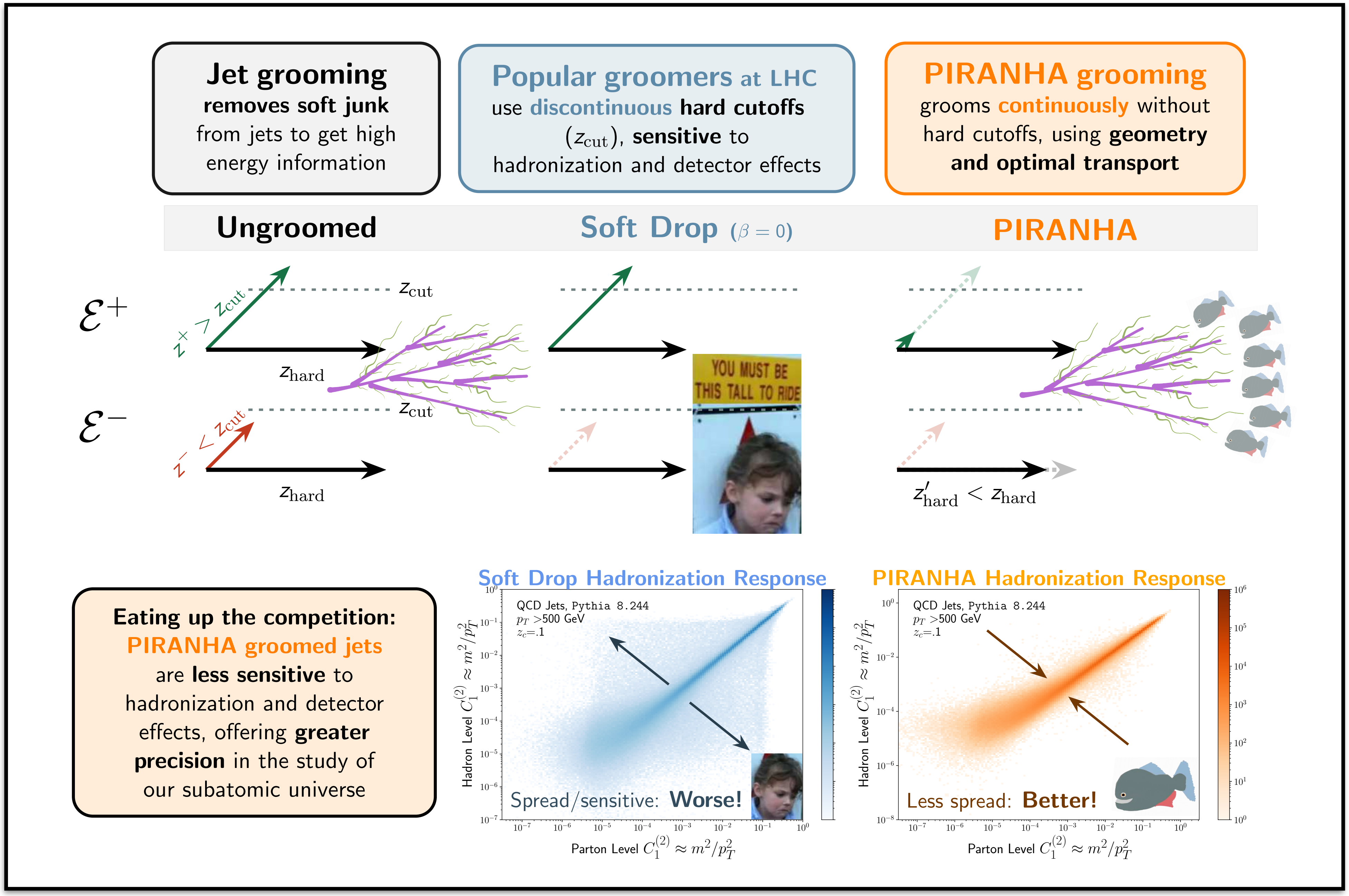


[JDT, Van Tilburg, JHEP 2011, JHEP 2012;
rephrased in the language of Komiske, Metodiev, JDT, PRL 2019]



Pileup and Infrared Radiation AnNiHilAtion

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



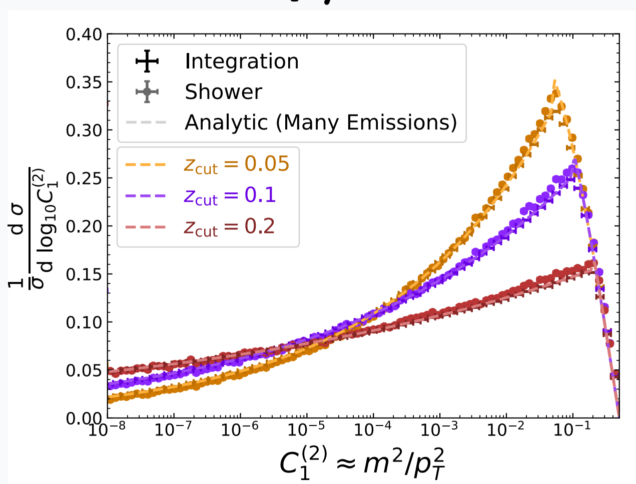
[Slides from Sam Alipour-fard]
[Alipour-fard, Komiske, Metodiev, JDT, in progress]

Pileup and Infrared Radiation AnNiHilAtion

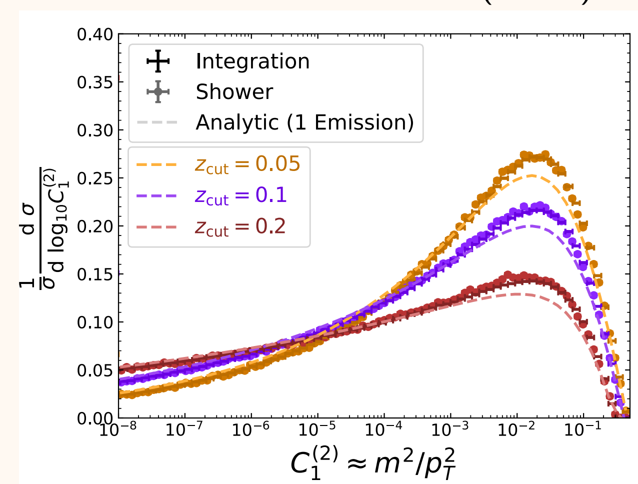
Recursive Safe Subtraction: tree-based approx. to optimal transport grooming

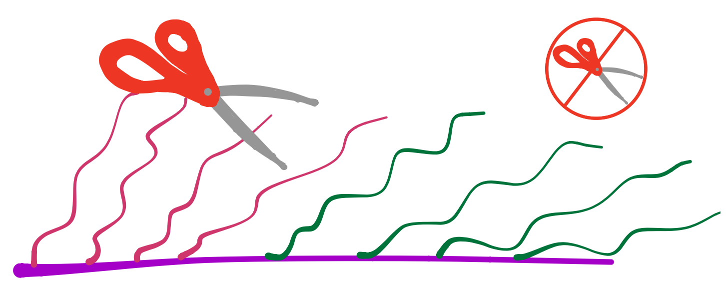
Fixed coupling, **multiple emission** calculations:

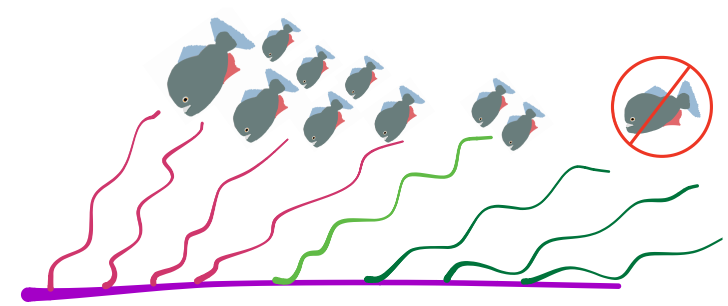
Soft Drop/mMDT



PIRANHA-RSS $(f = 1)$







Sharp cutoff $\rightarrow$ kink

No sharp cutoff $\rightarrow$ smooth

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