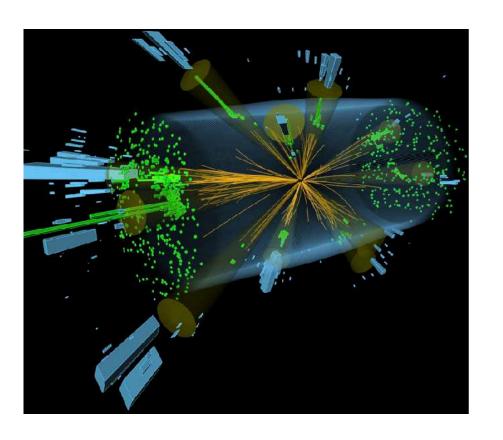
Optimizing Particle Physics with Machine Learning

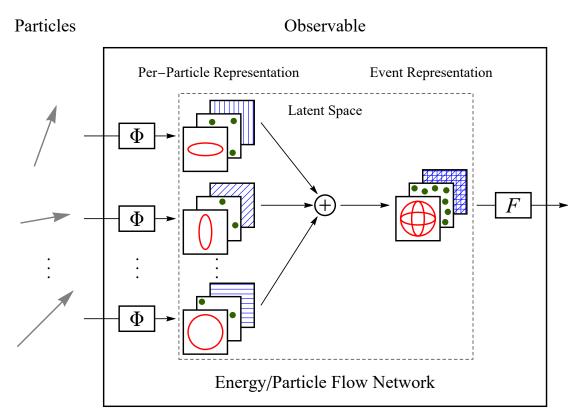
Patrick T. Komiske III

Massachusetts Institute of Technology
Center for Theoretical Physics
NSF AI Institute for Artificial Intelligence and Fundamental Interactions

MIT Lincoln Laboratory

Groups 41 & 89 Joint Seminar



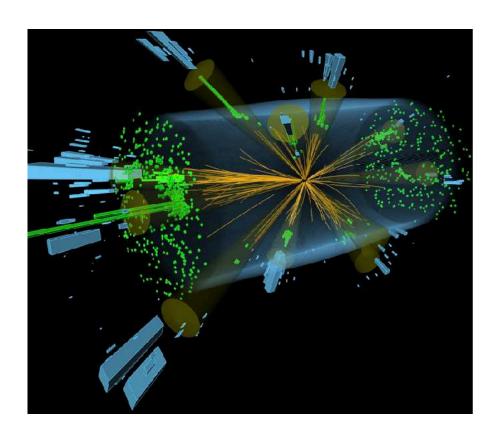


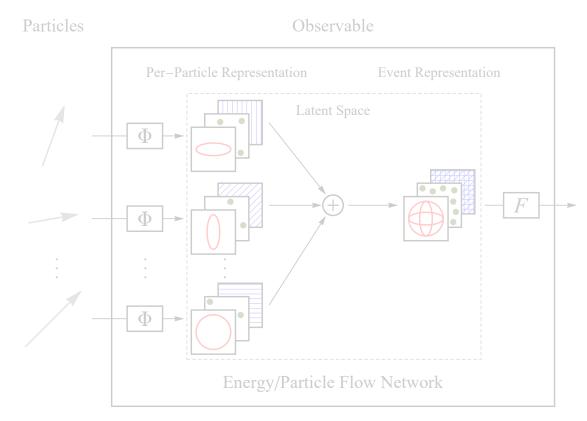


Particle Physics Fundamentals

Architectures for Colliders

Statistical Deconvolution







Particle Physics Fundamentals

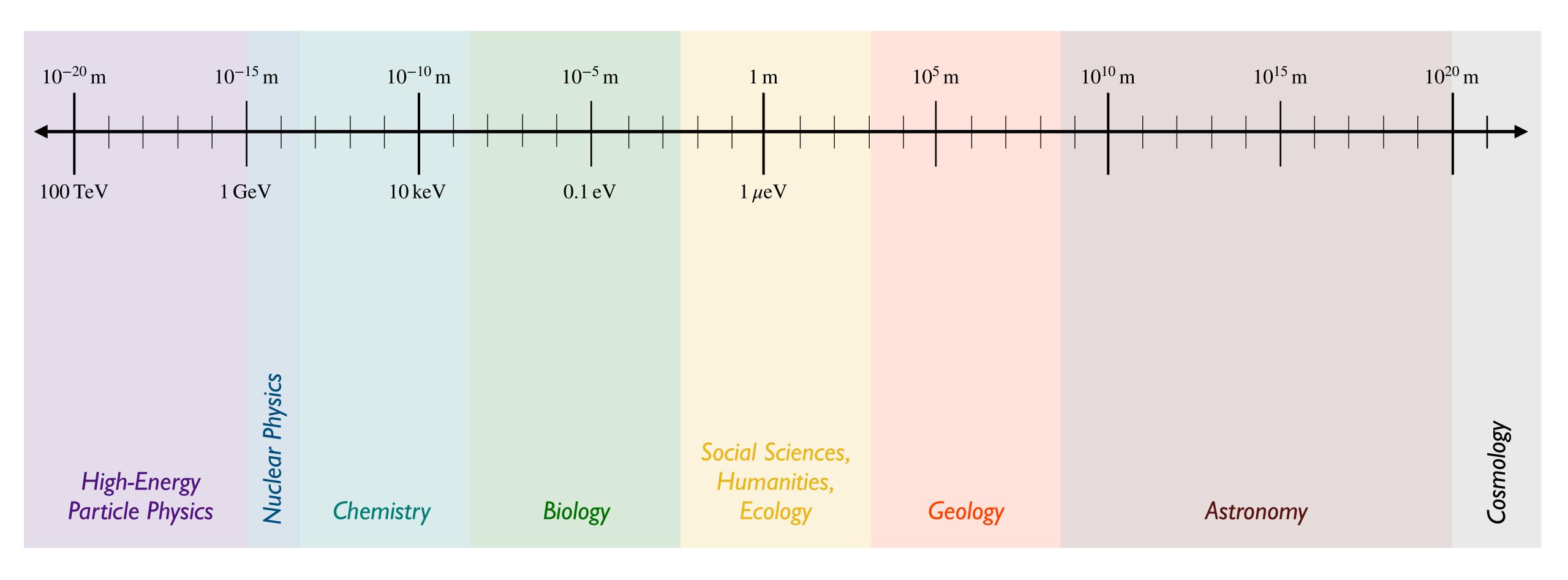
Why do we collide particles at ultra-high energies?

What are some outstanding challenges that ML can help address?

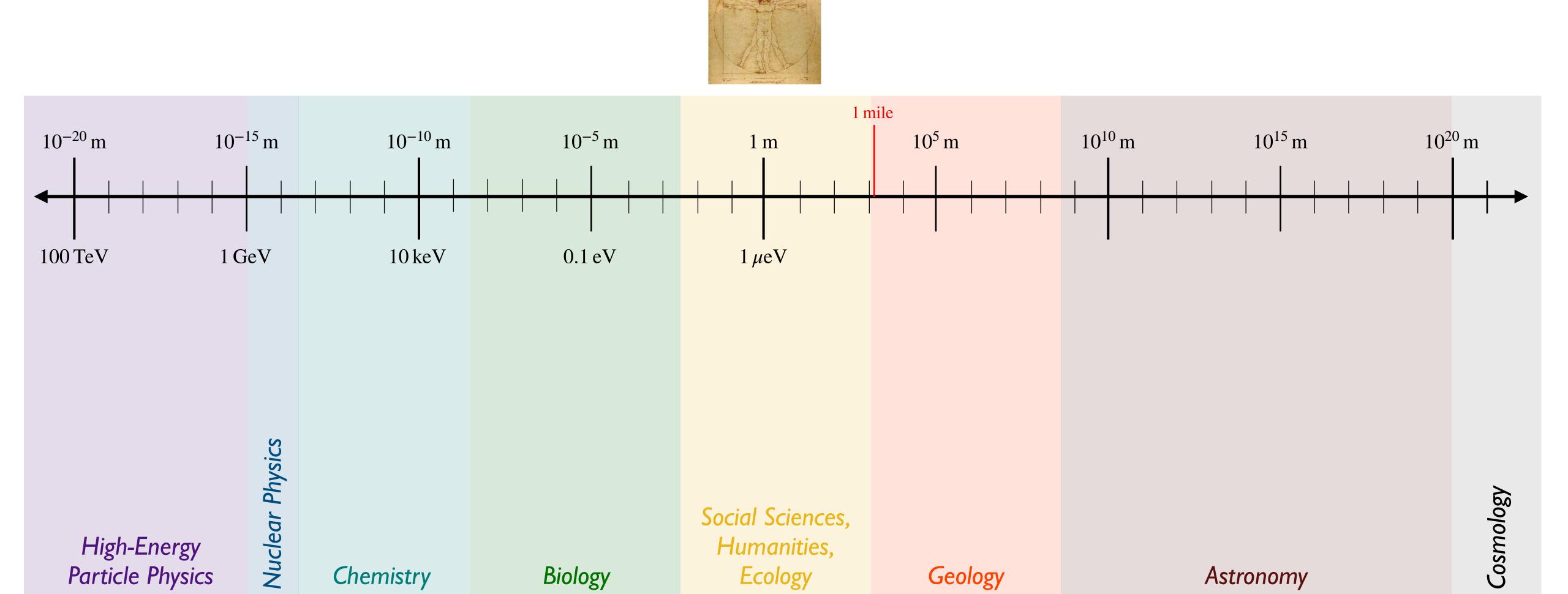
Architectures for Colliders

Statistical Deconvolution

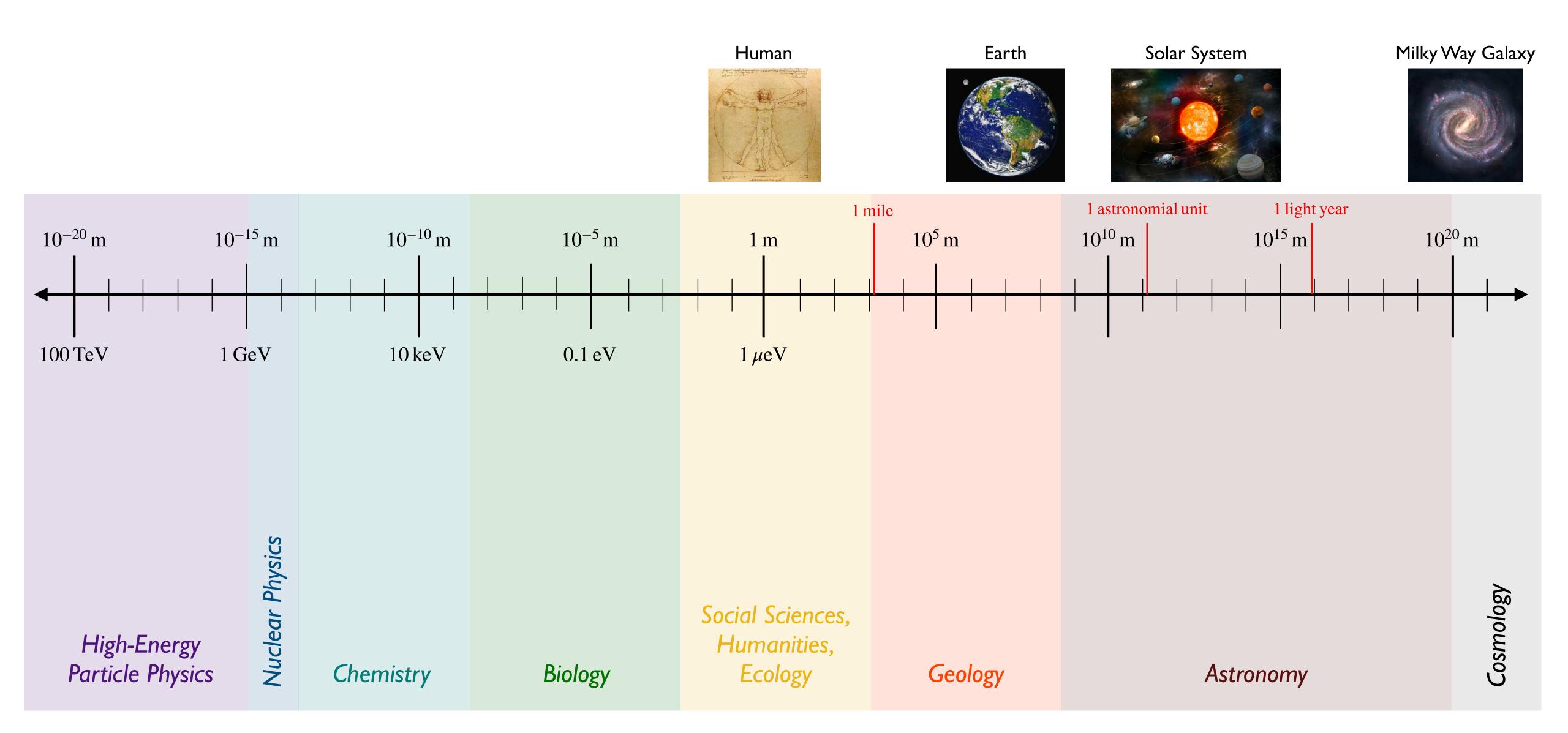
Einstein-Planck Equation:
$$E = \frac{hc}{\lambda}$$

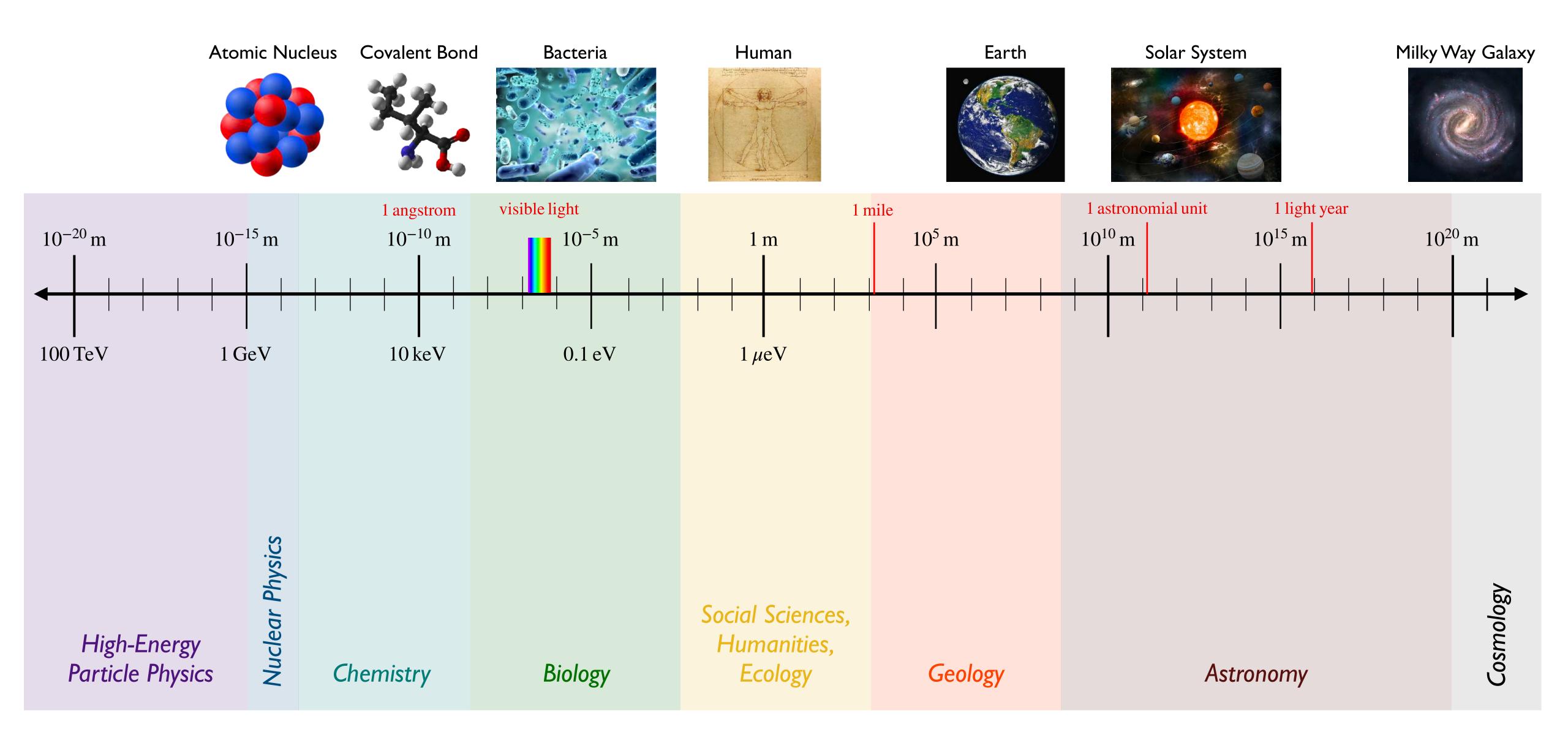


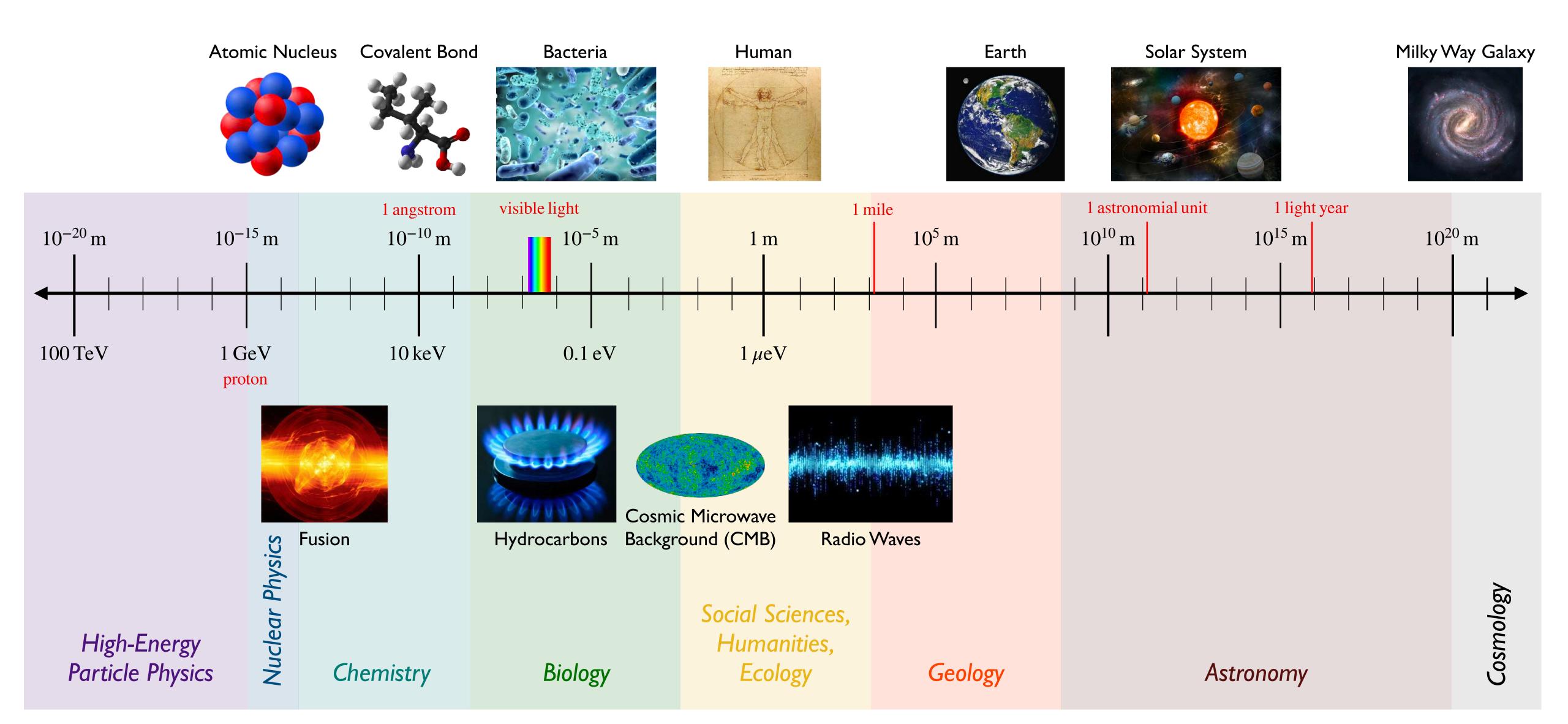
Einstein-Planck Equation: $E = \frac{hc}{\lambda}$

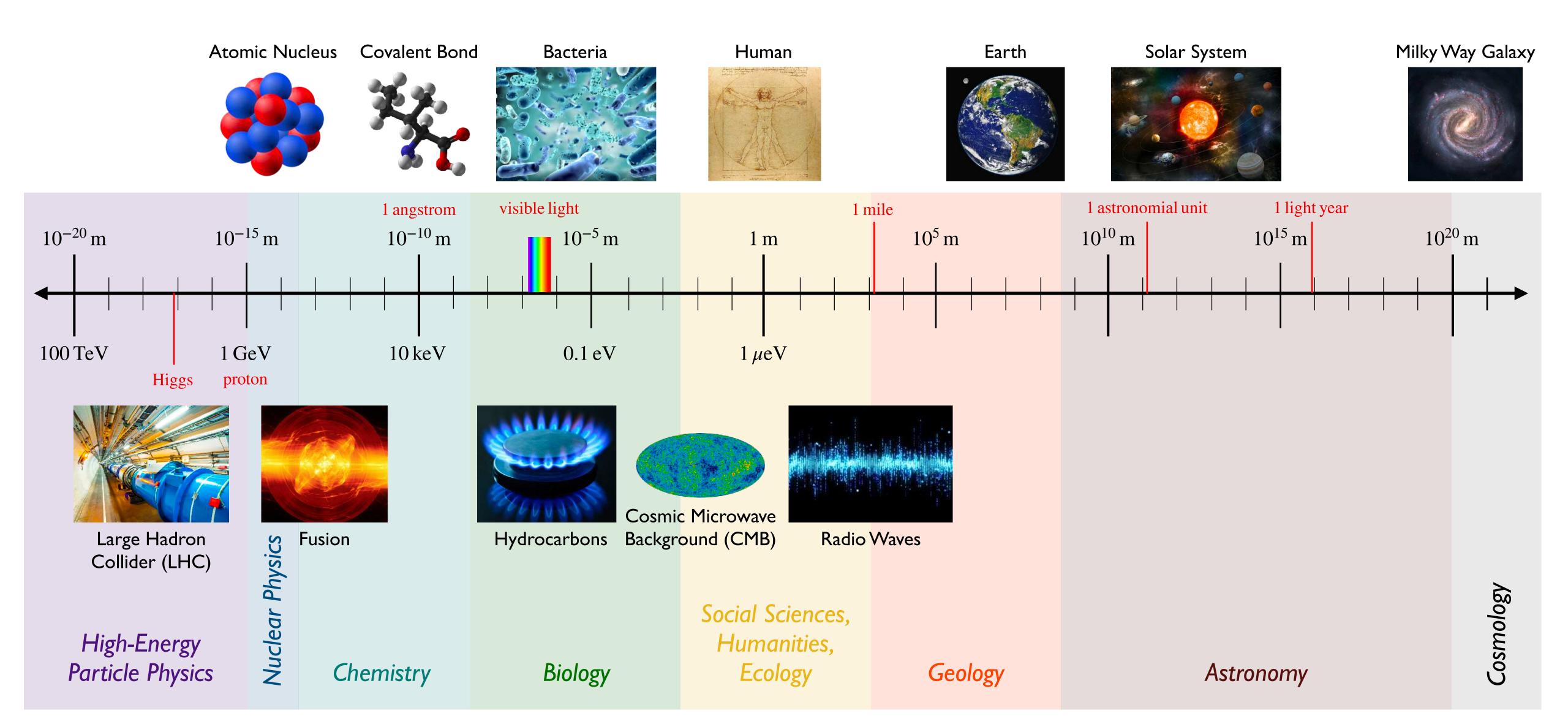


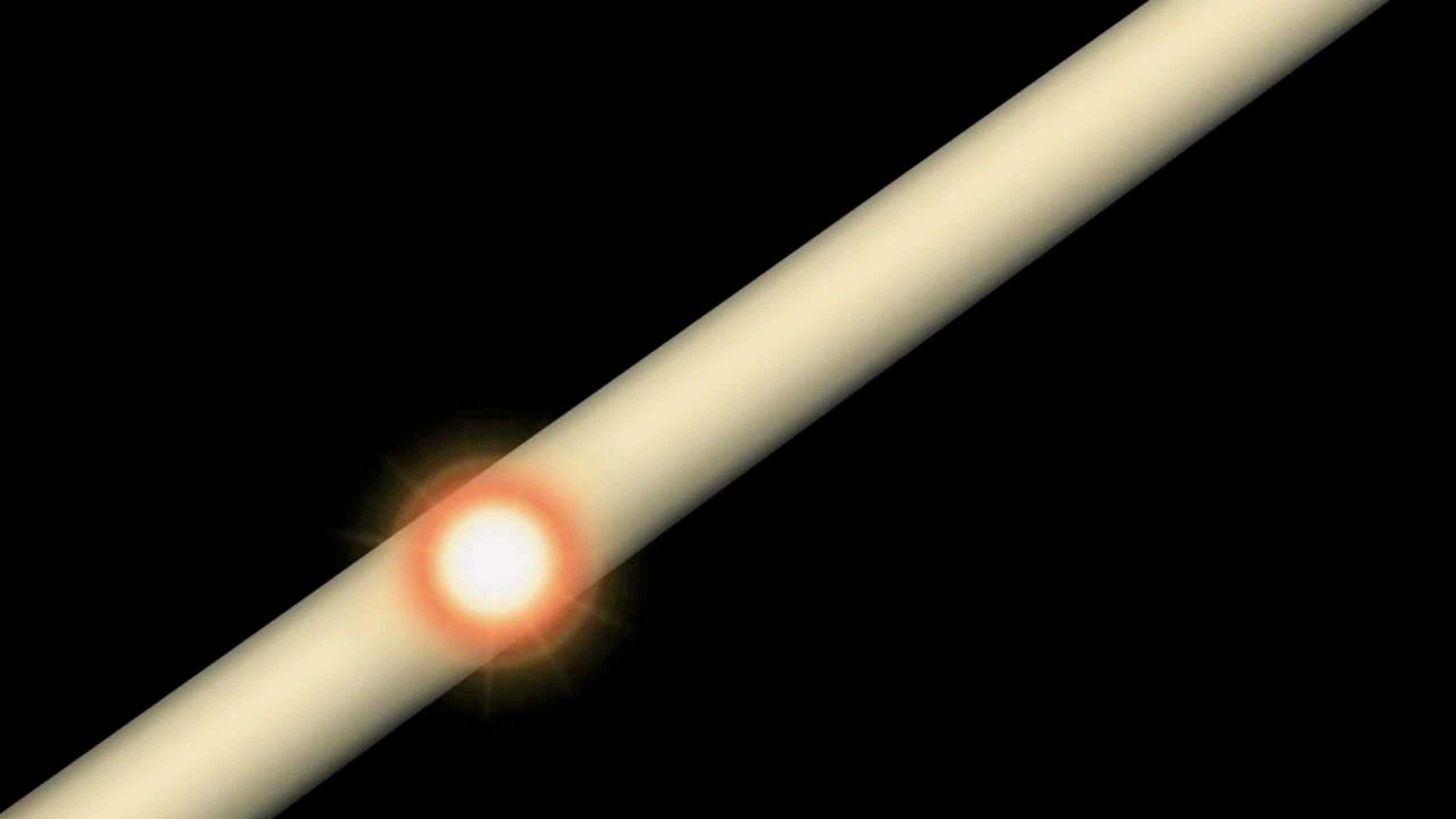
Human

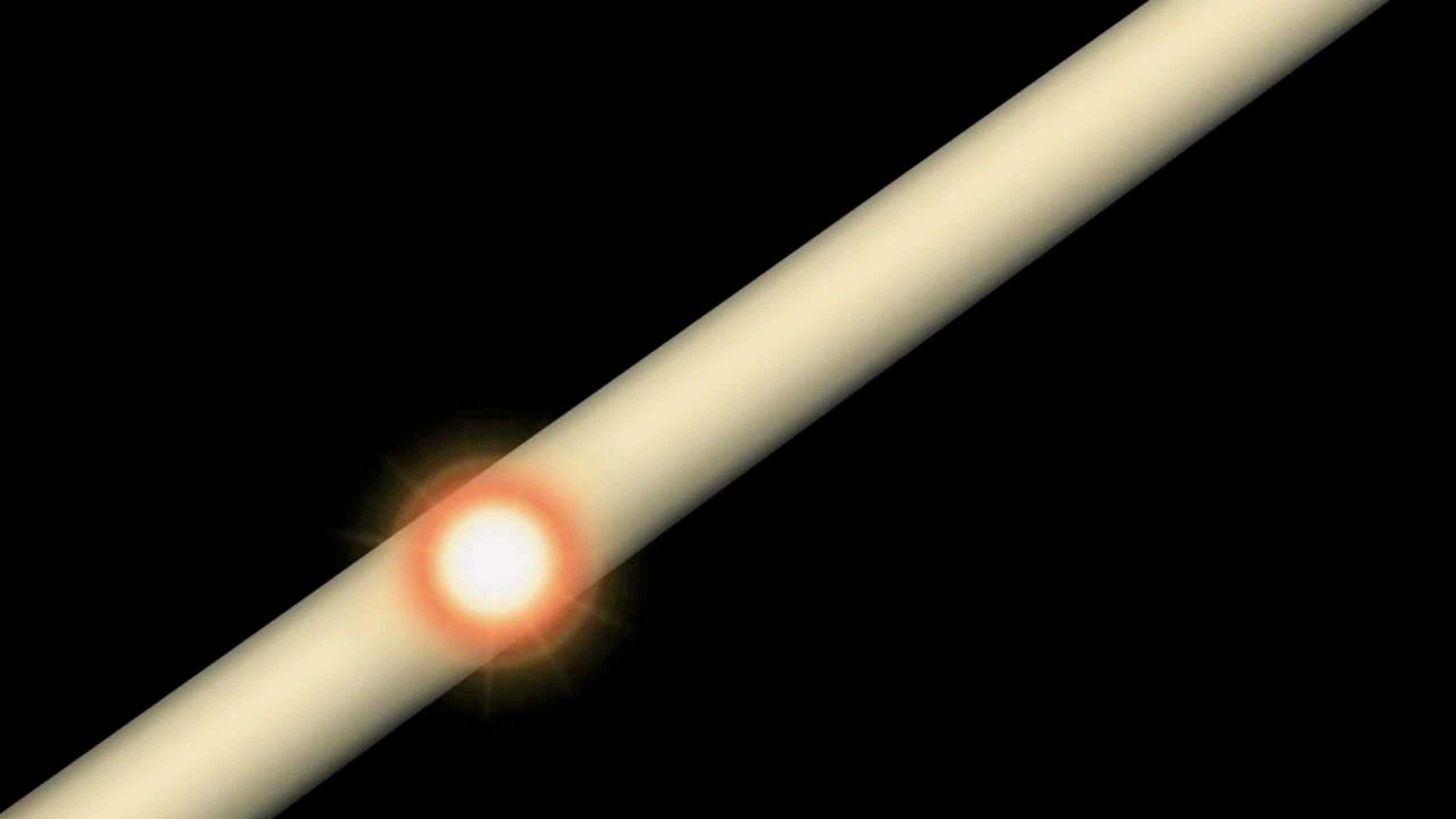






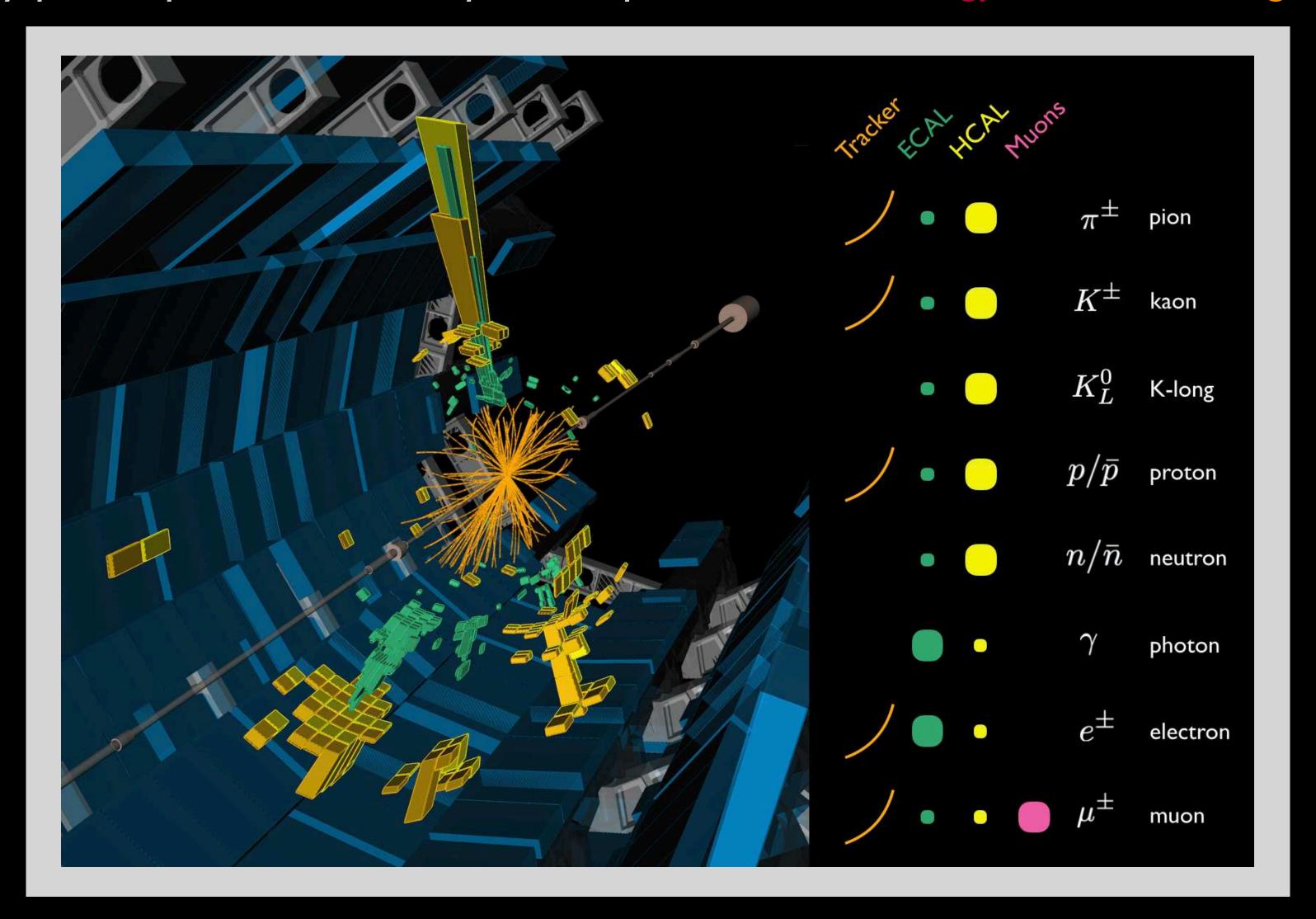


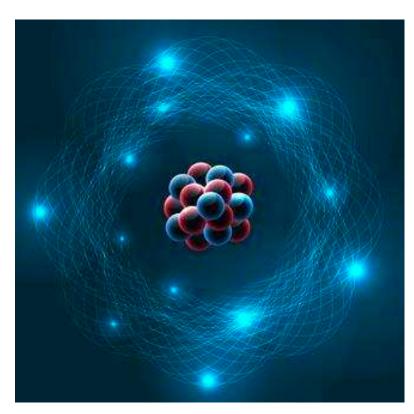




Events at the LHC

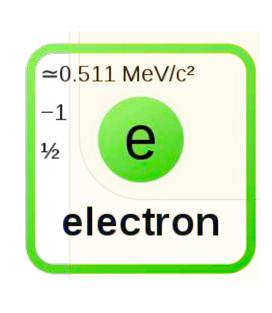
High-energy proton-proton collisions produce particles with energy, direction, charge, and flavor



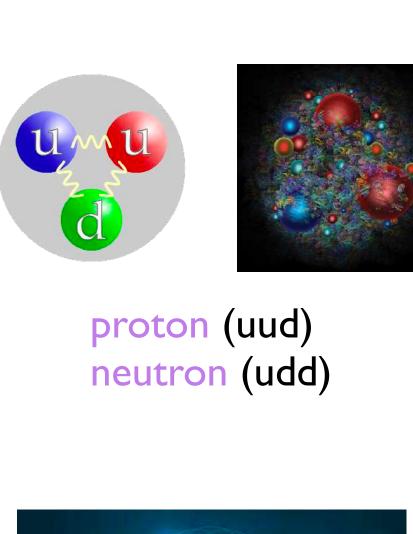


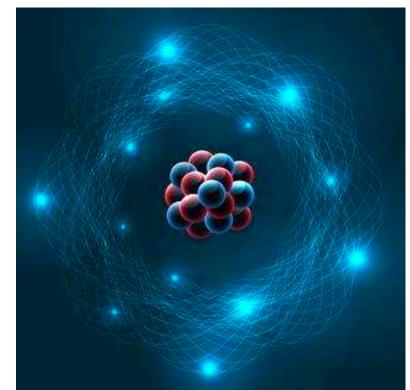
Atomic ingredients

- nucleus of protons and neutrons
- electron cloud around nucleus
- bound by electromagnetism



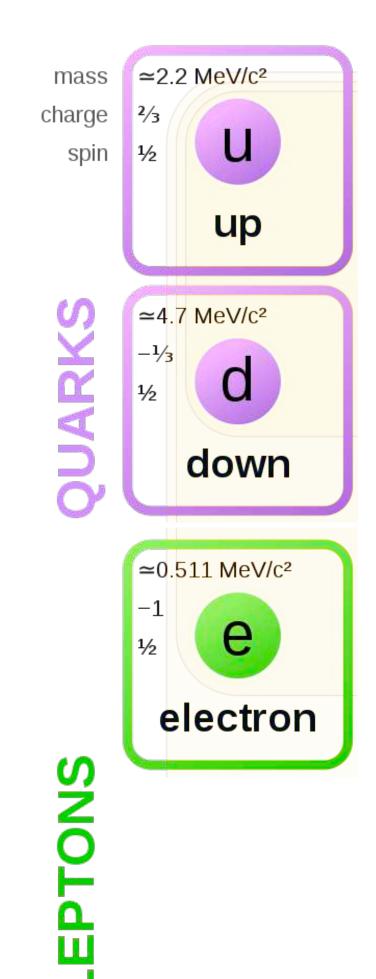




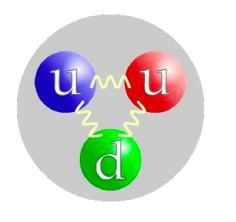


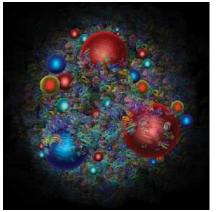
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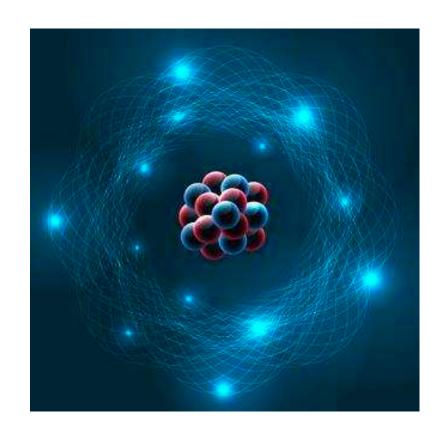






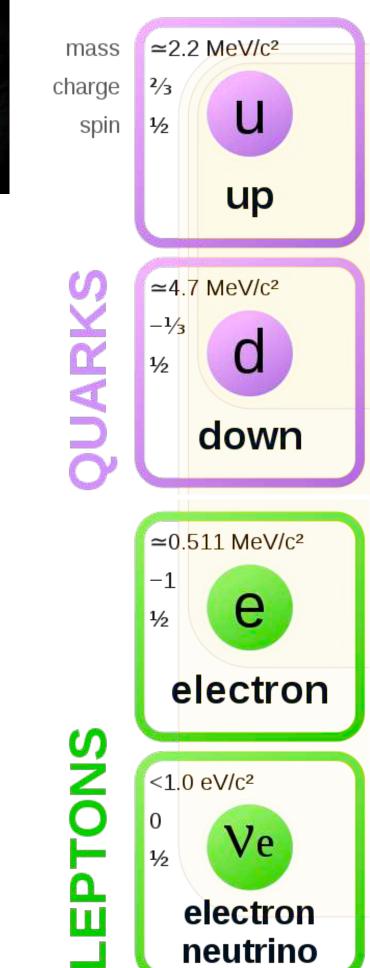


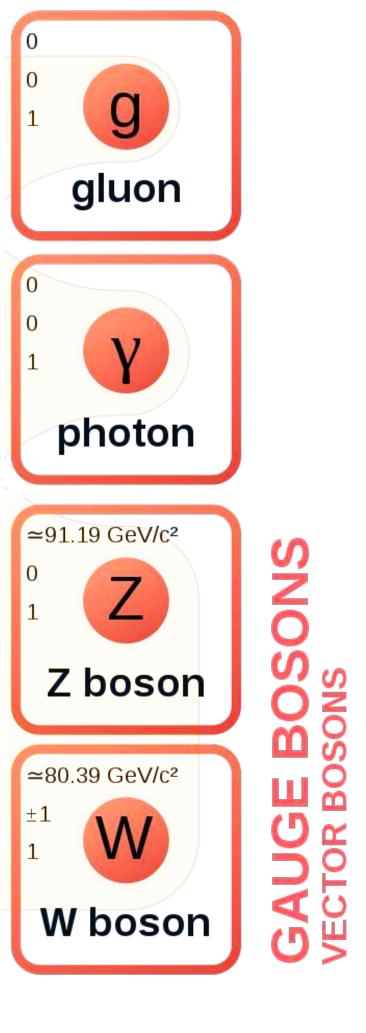
proton (uud)
neutron (udd)



Atomic ingredients

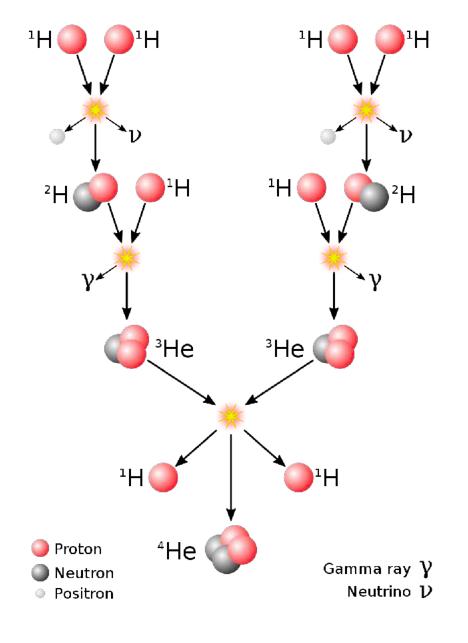
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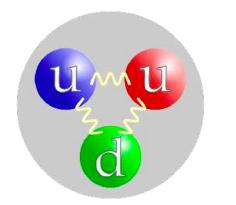


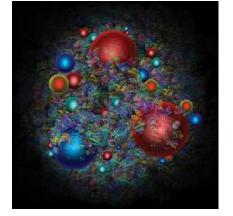


Solar nuclear fusion

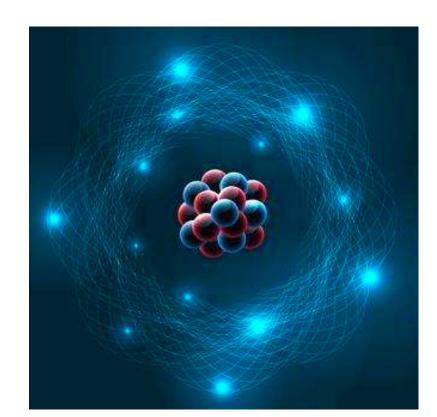
- protons first fuse into deuterium via weak force (a.k.a. W boson)
- ~9 billion years for average proton to fuse





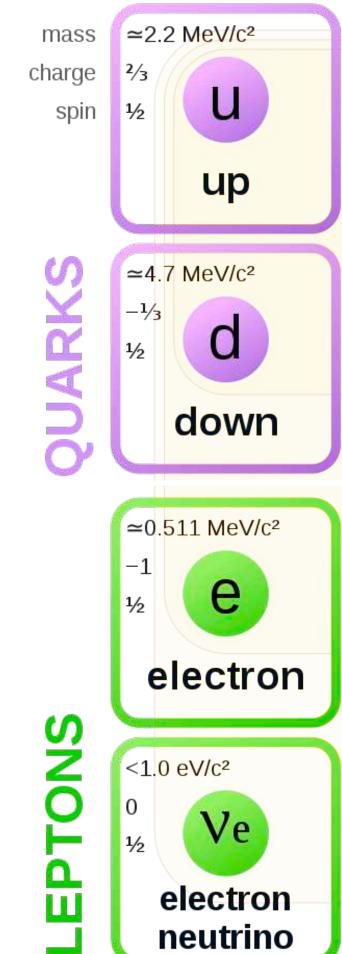


proton (uud) neutron (udd)



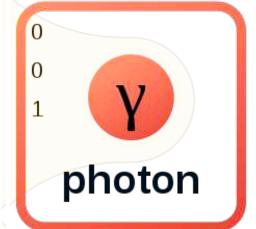
Atomic ingredients

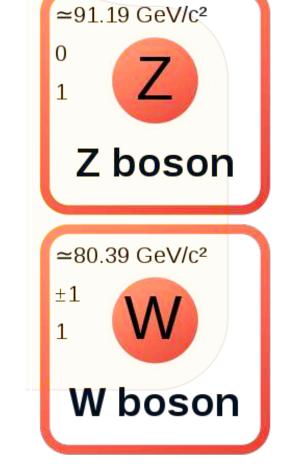
- nucleus of protons and neutrons
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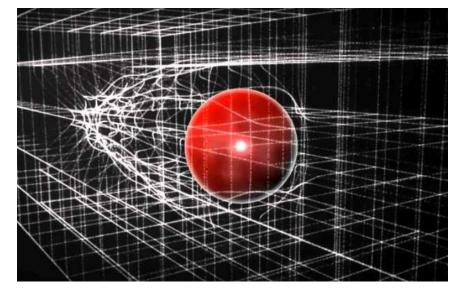








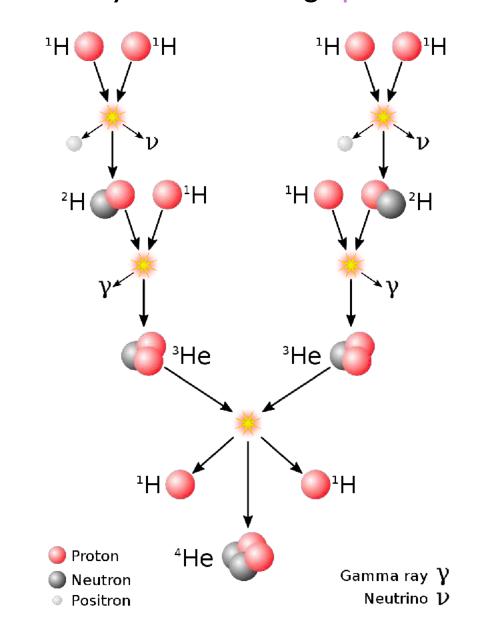




Particle mass comes from interaction with Higgs field

Solar nuclear fusion

- protons first fuse into deuterium via weak force (a.k.a. W boson)
- ~9 billion years for average proton to fuse



(fermions)

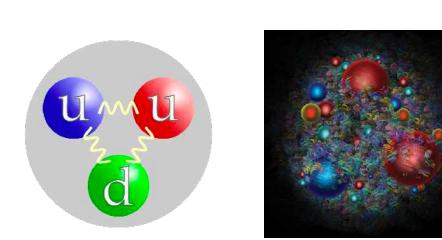
charm

strange

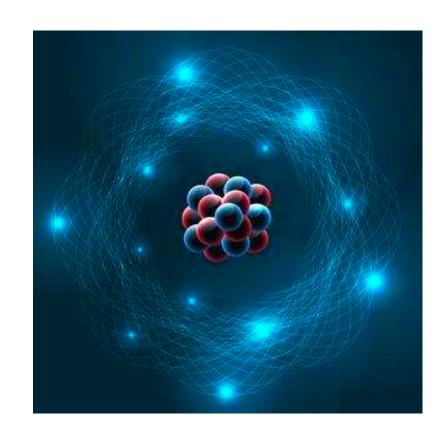
≃105.66 MeV/c²

≃1.28 GeV/c²

≃96 MeV/c²

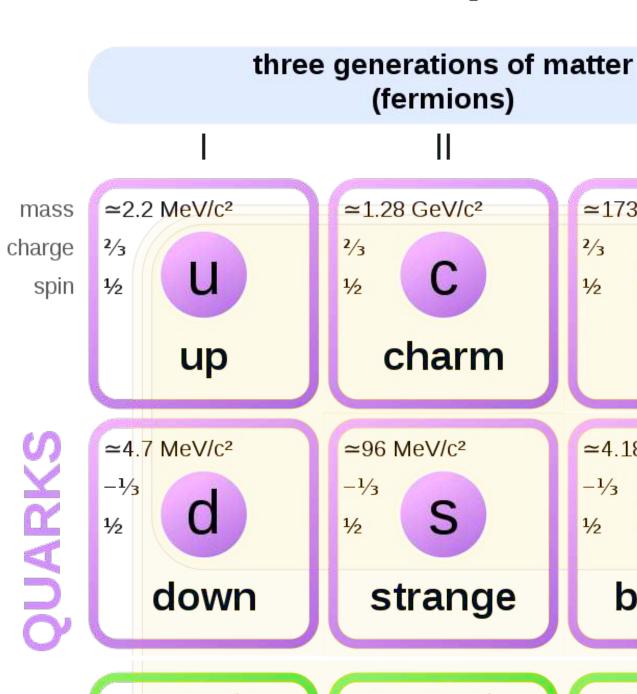


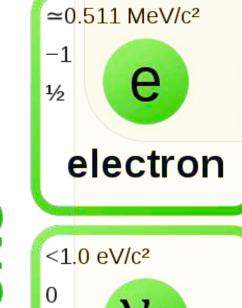
proton (uud) neutron (udd)

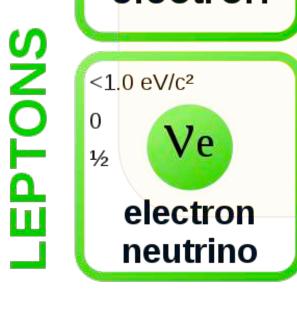


Atomic ingredients

- nucleus of protons and neutrons
- electron cloud around nucleus
- bound by electromagnetism











Ш

top

bottom

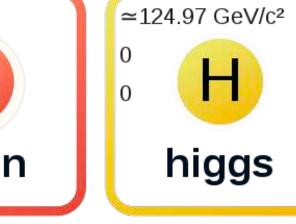
≃1.7768 GeV/c²

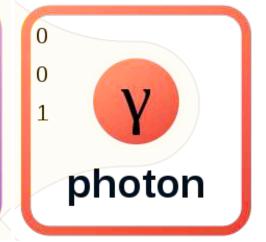
≃4.18 GeV/c²

≃173.1 GeV/c²

interactions / force carriers (bosons)





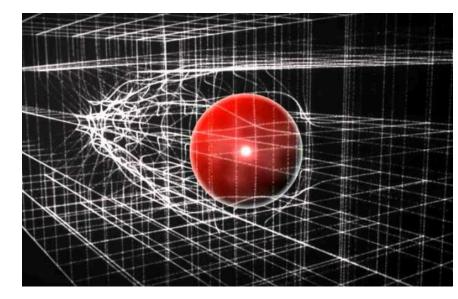


≃91.19 GeV/c²

W boson



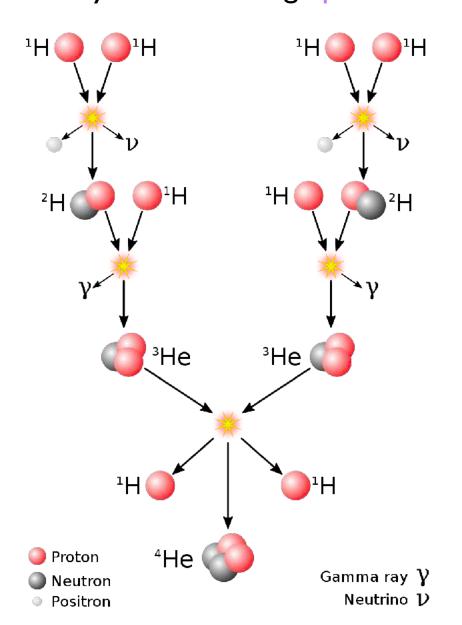




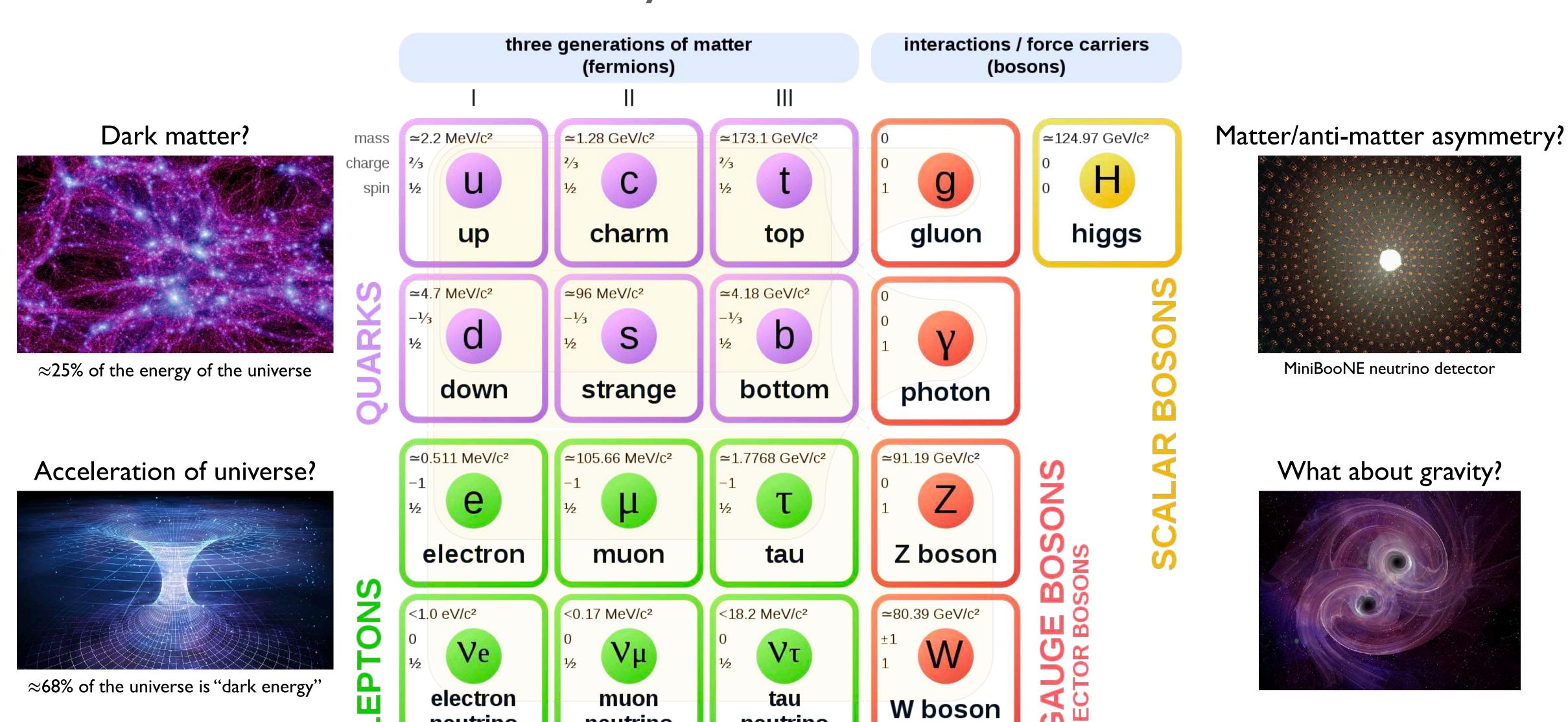
Particle mass comes from interaction with Higgs field

Solar nuclear fusion

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Standard Model of Particle Physics – Unanswered Questions

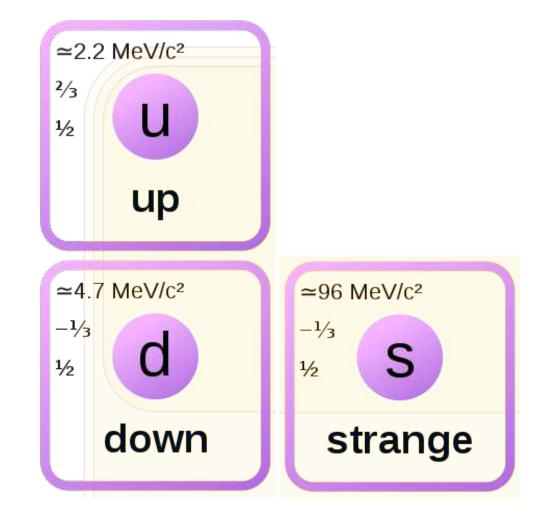


neutrino

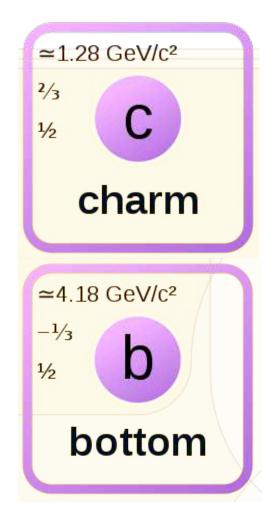
neutrino

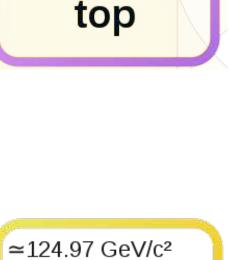
neutrino

Light quarks

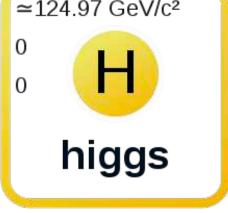


Intermediate quarks

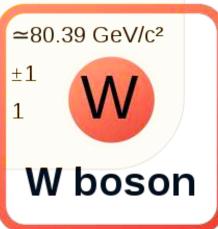




≃173.1 GeV/c²

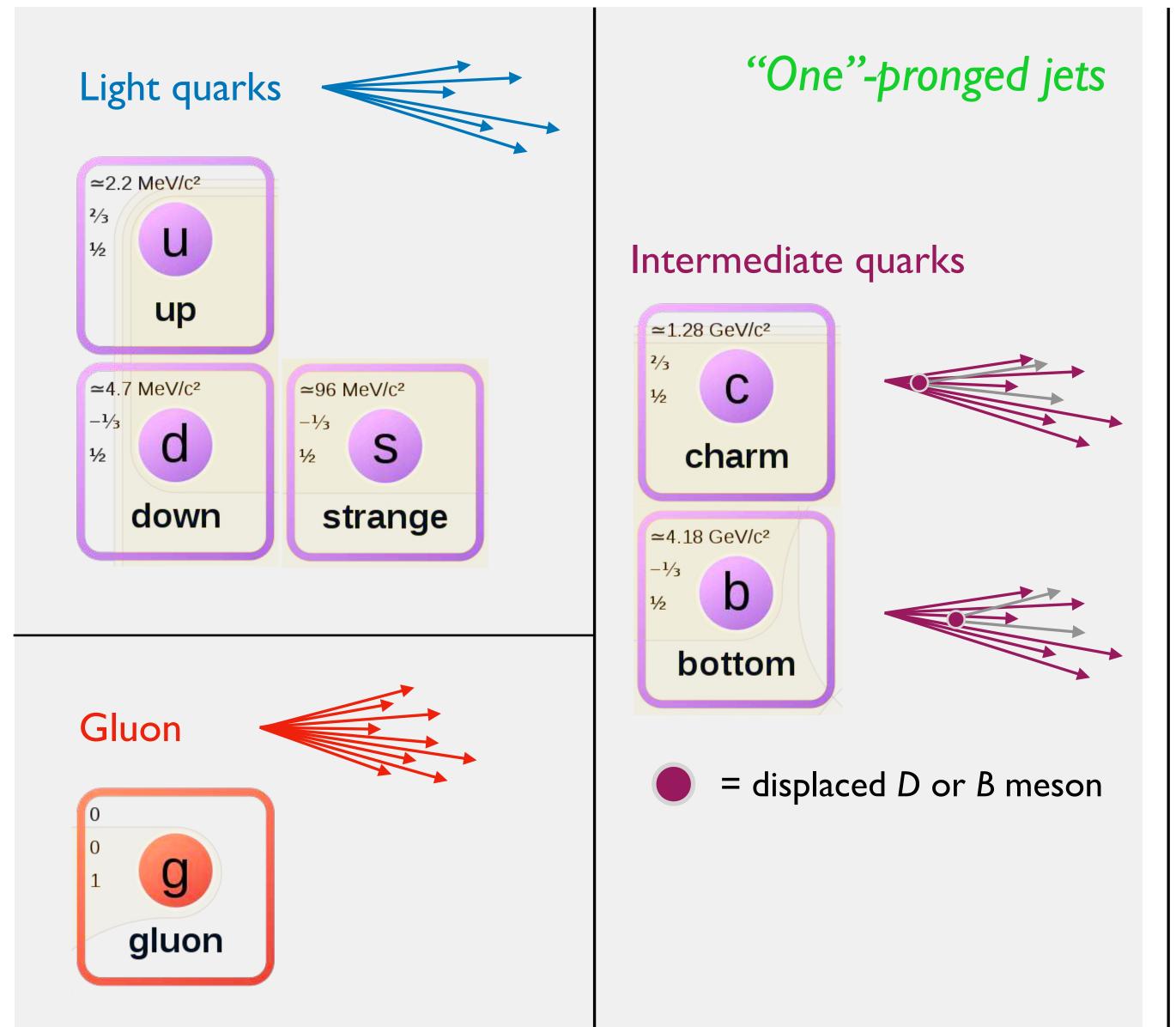


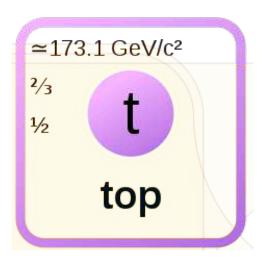




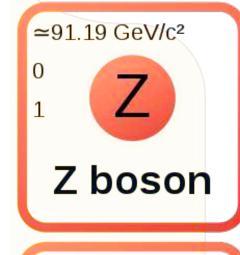
Gluon

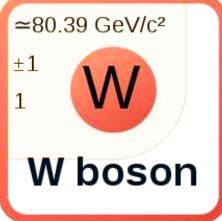


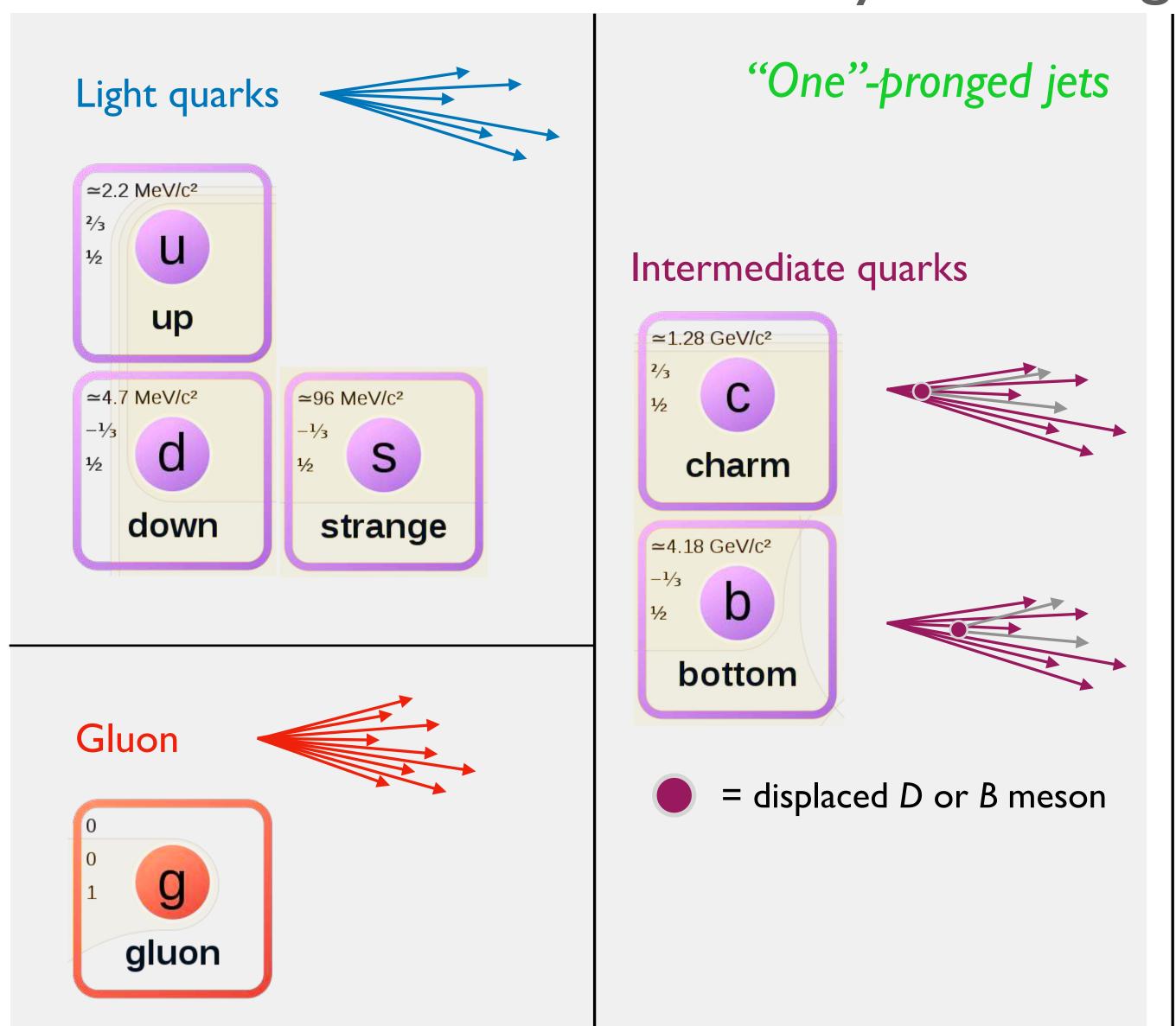


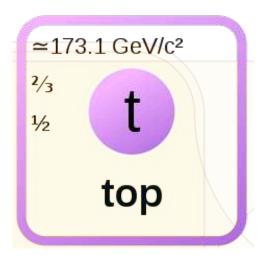


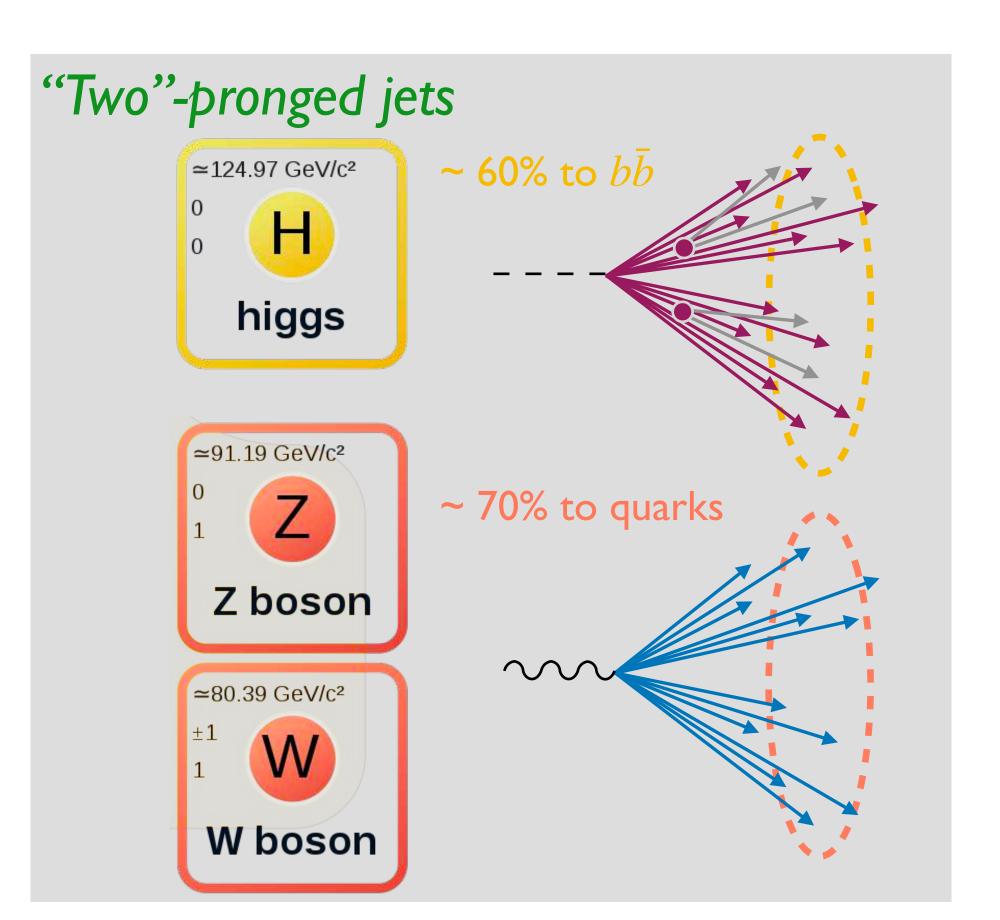


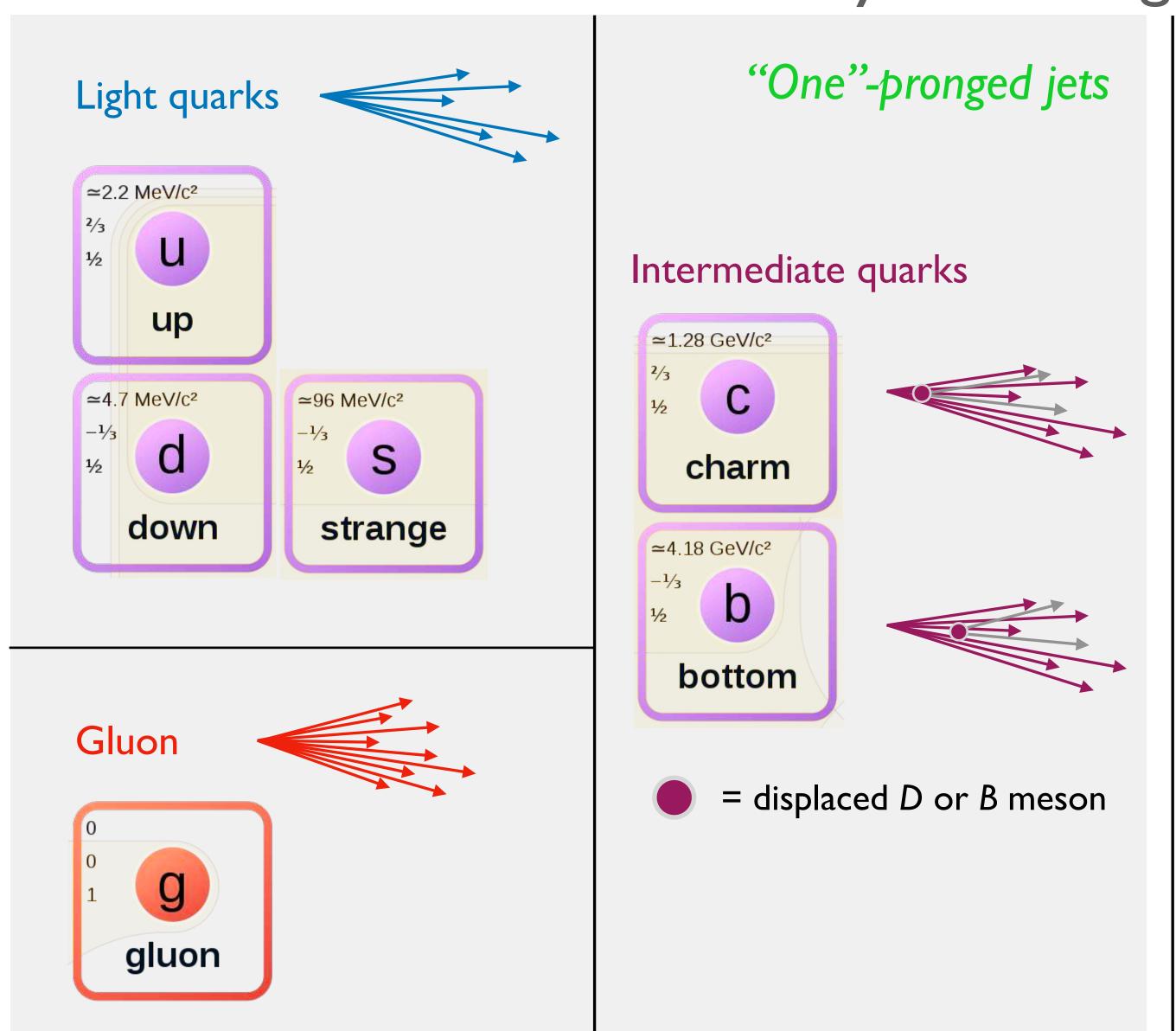


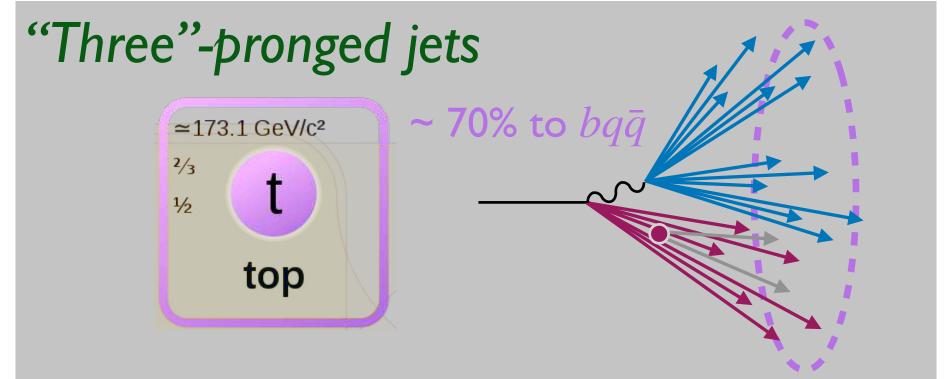


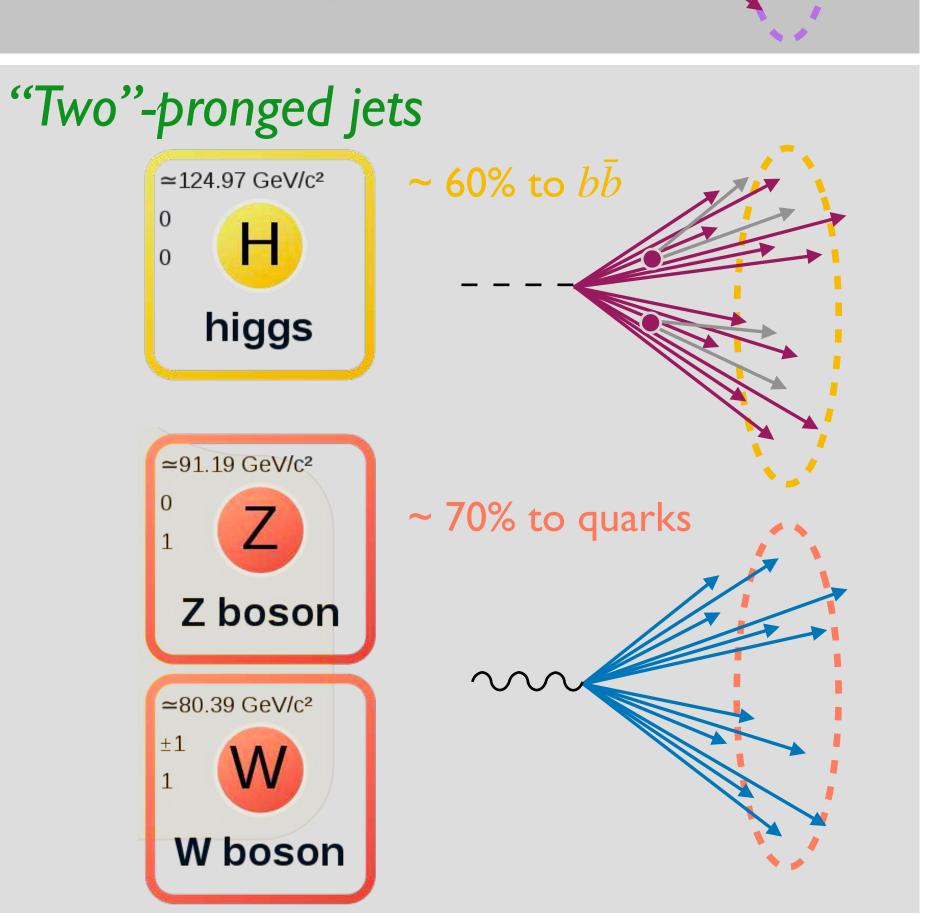




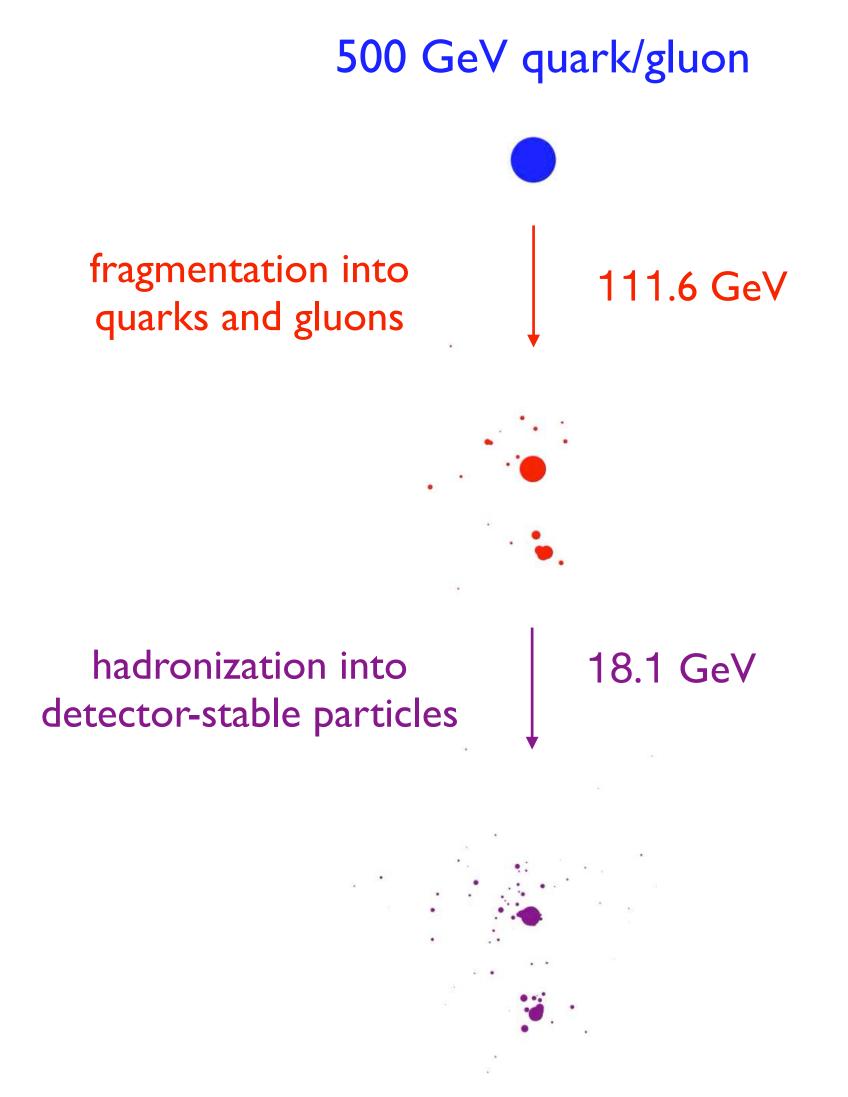


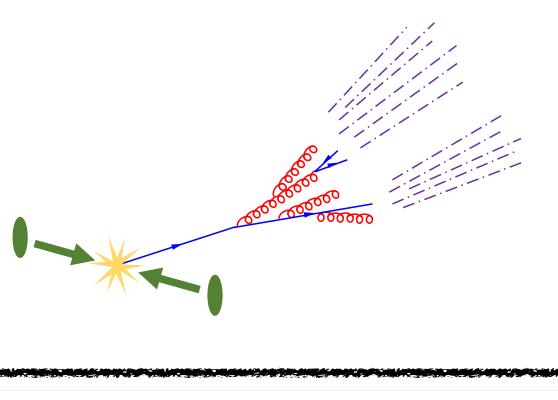


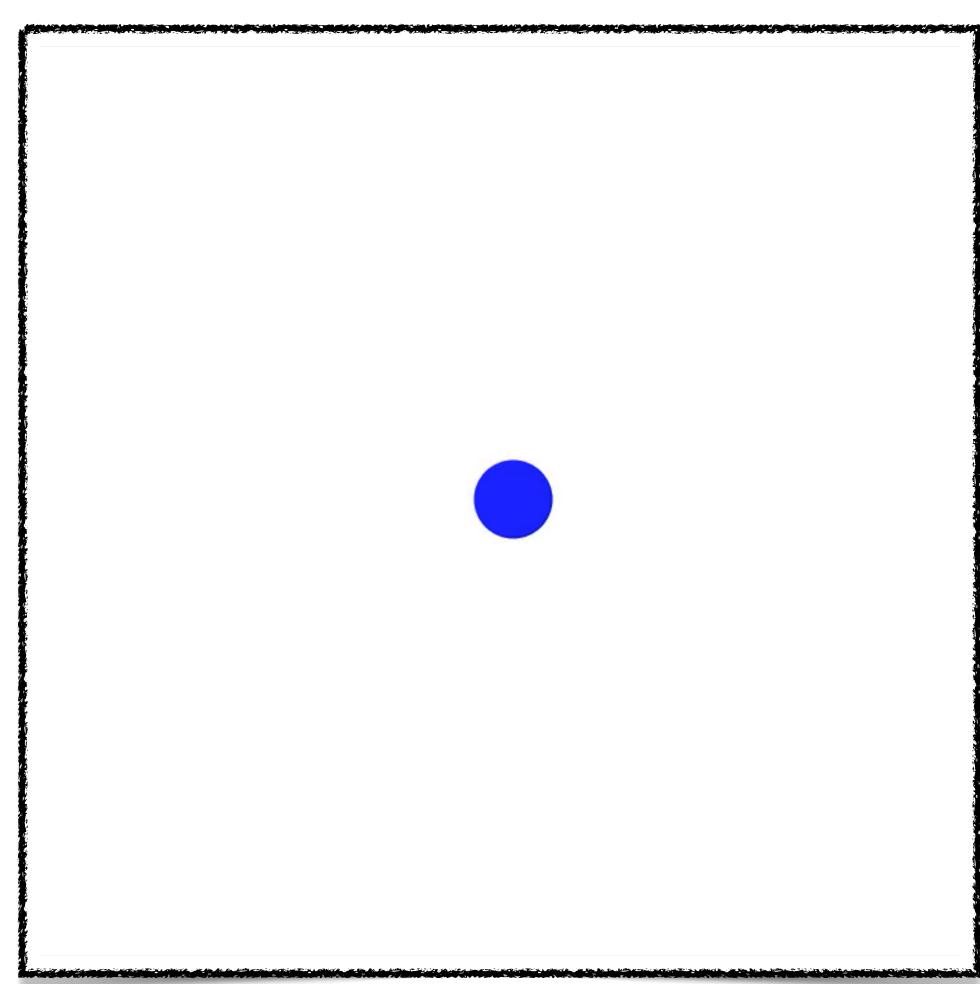




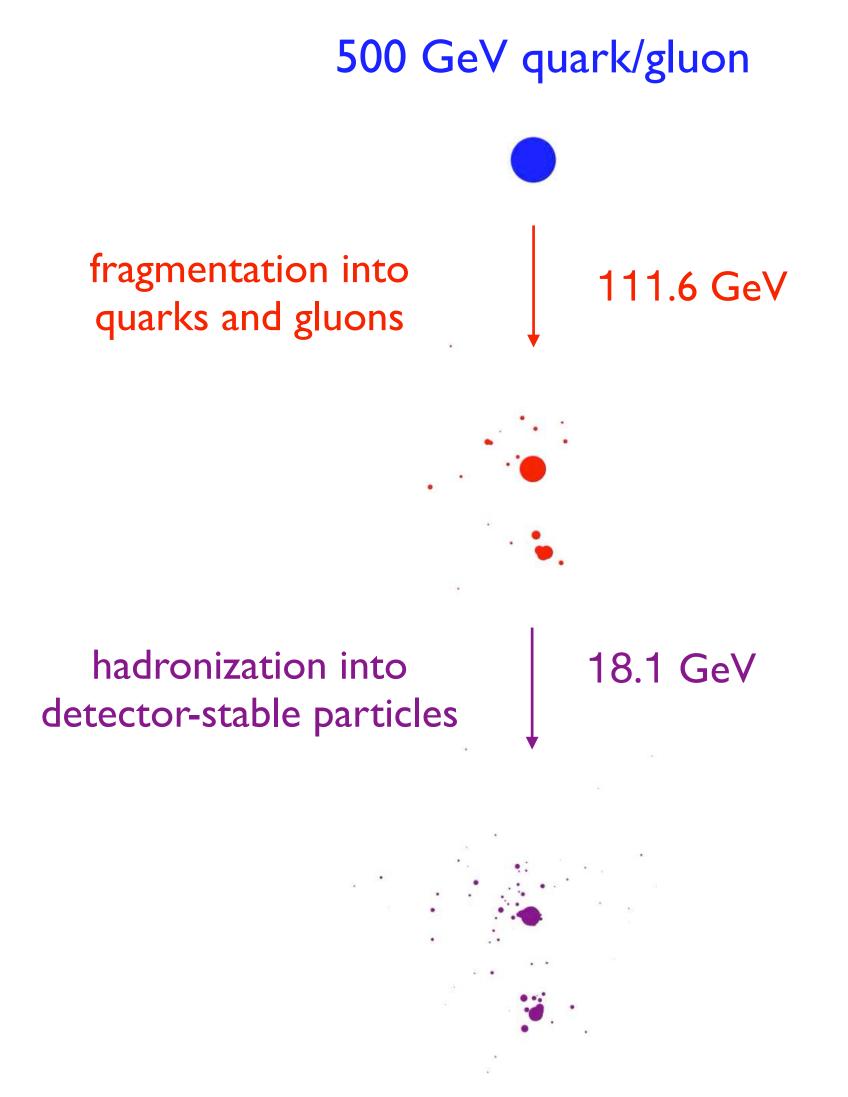
Visualizing Jet Formation – QCD Jets

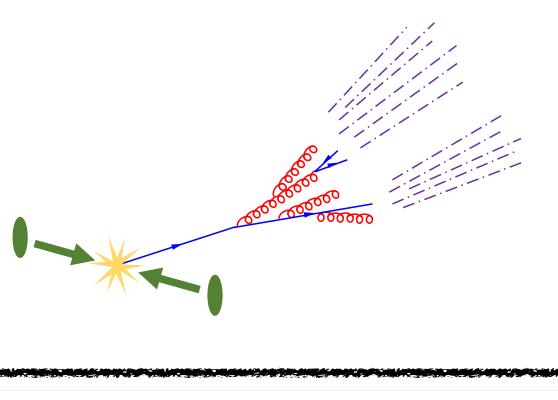


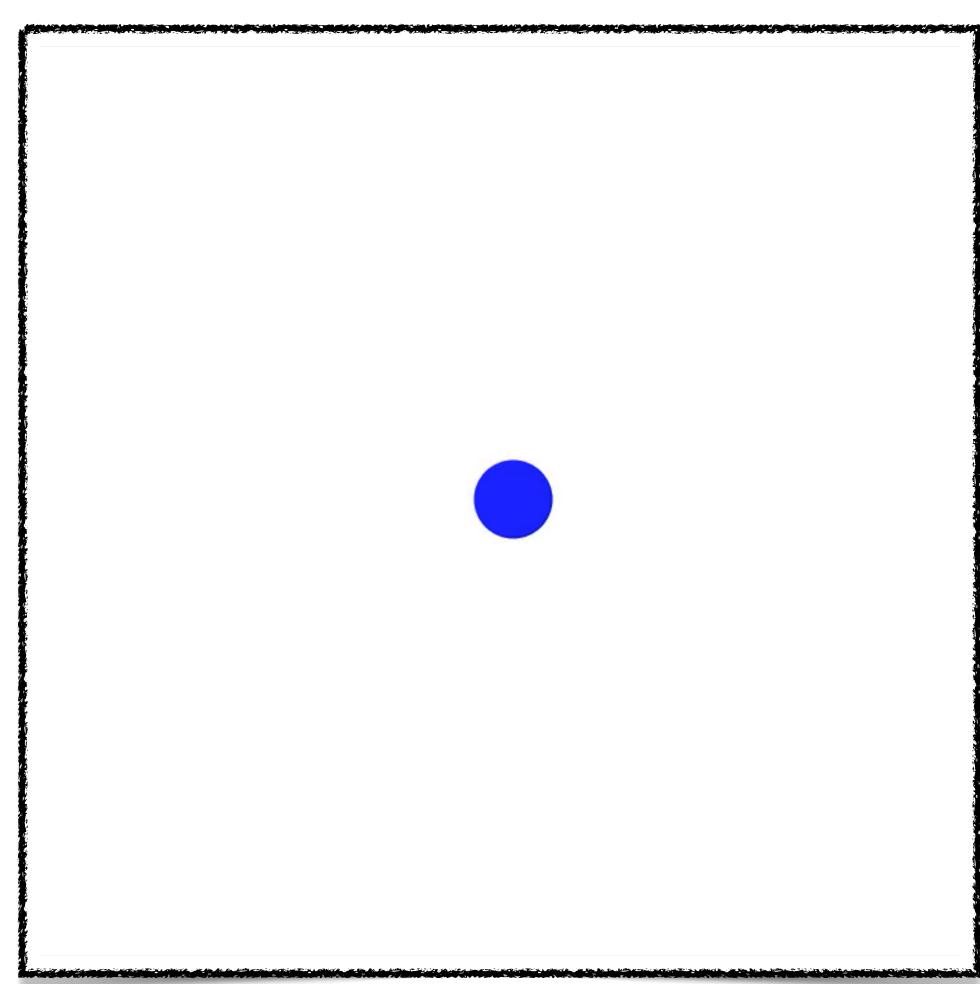




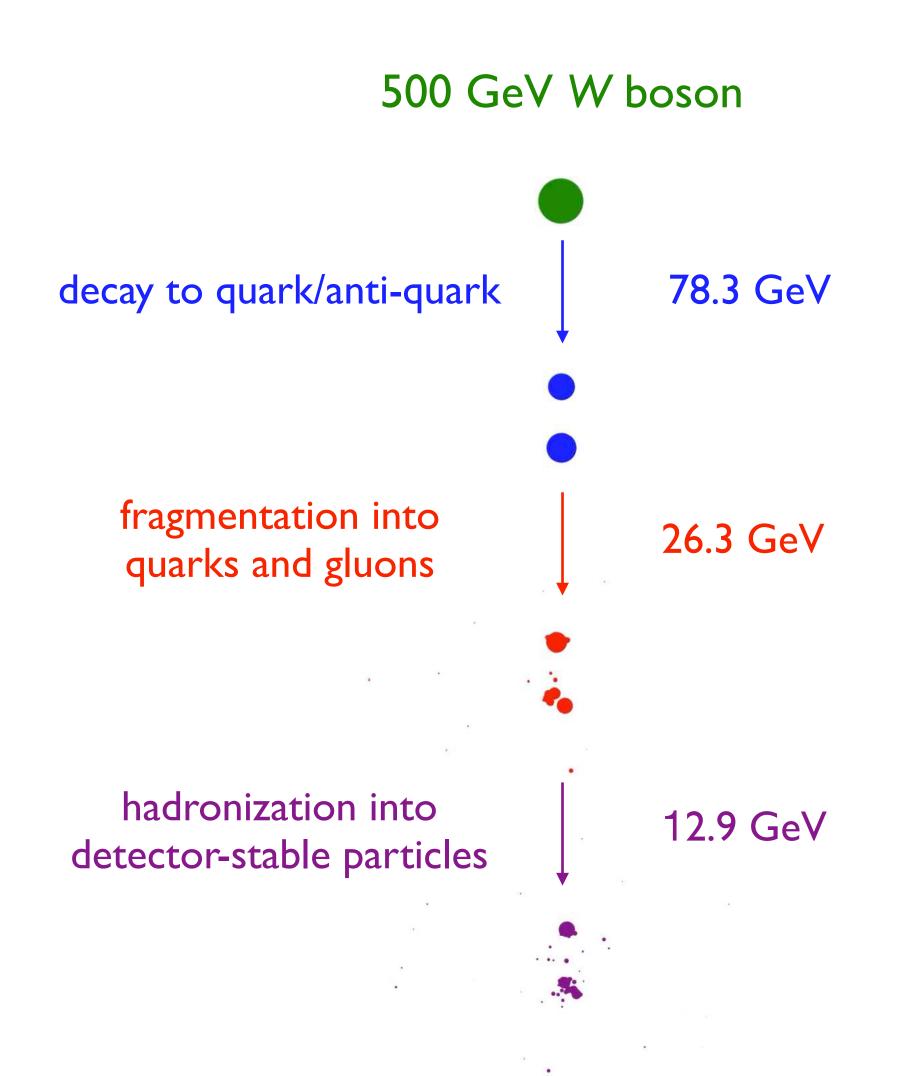
Visualizing Jet Formation – QCD Jets

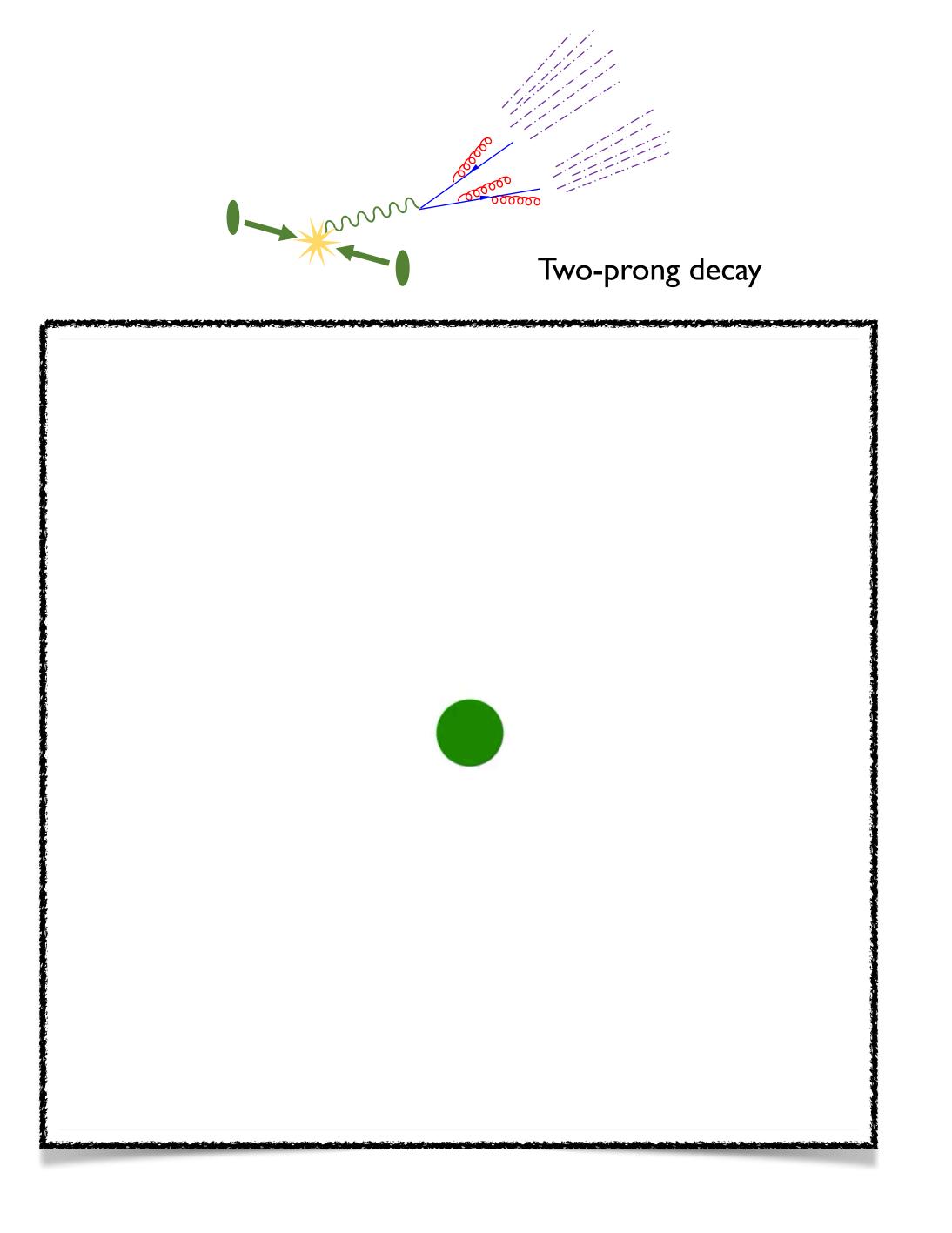




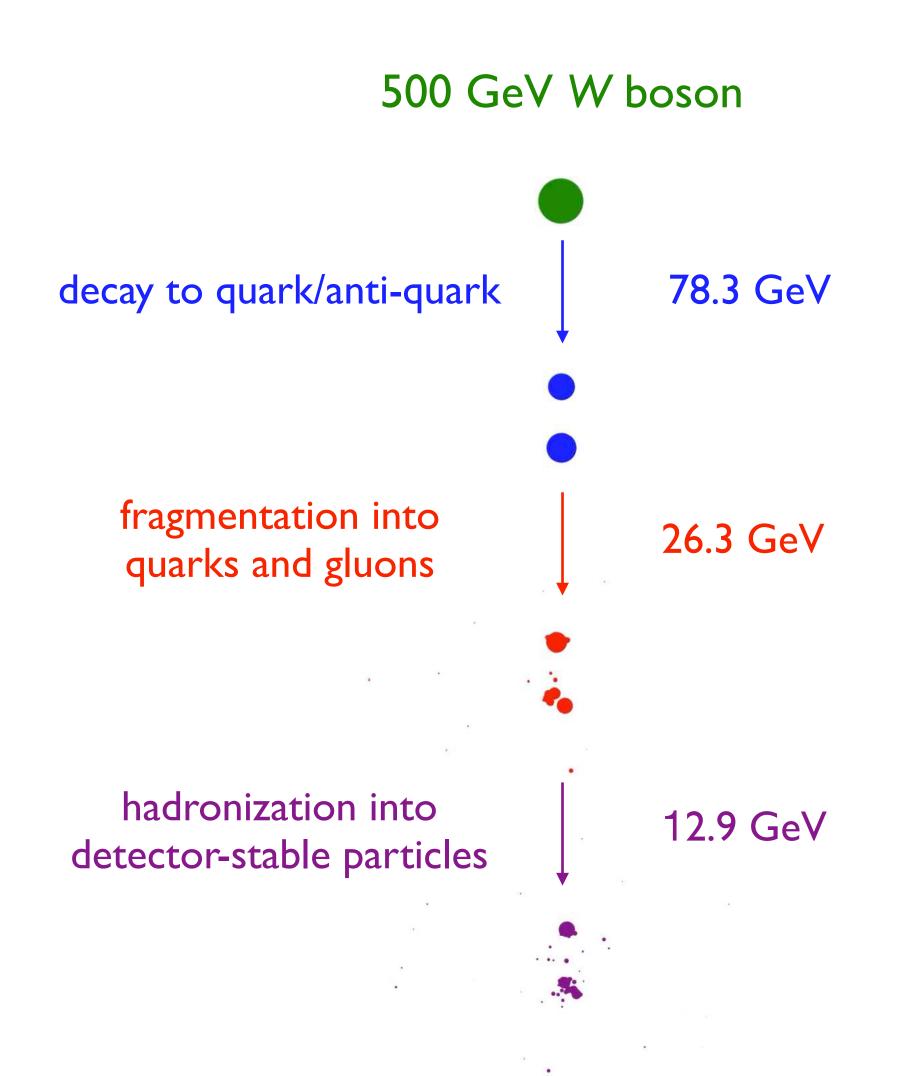


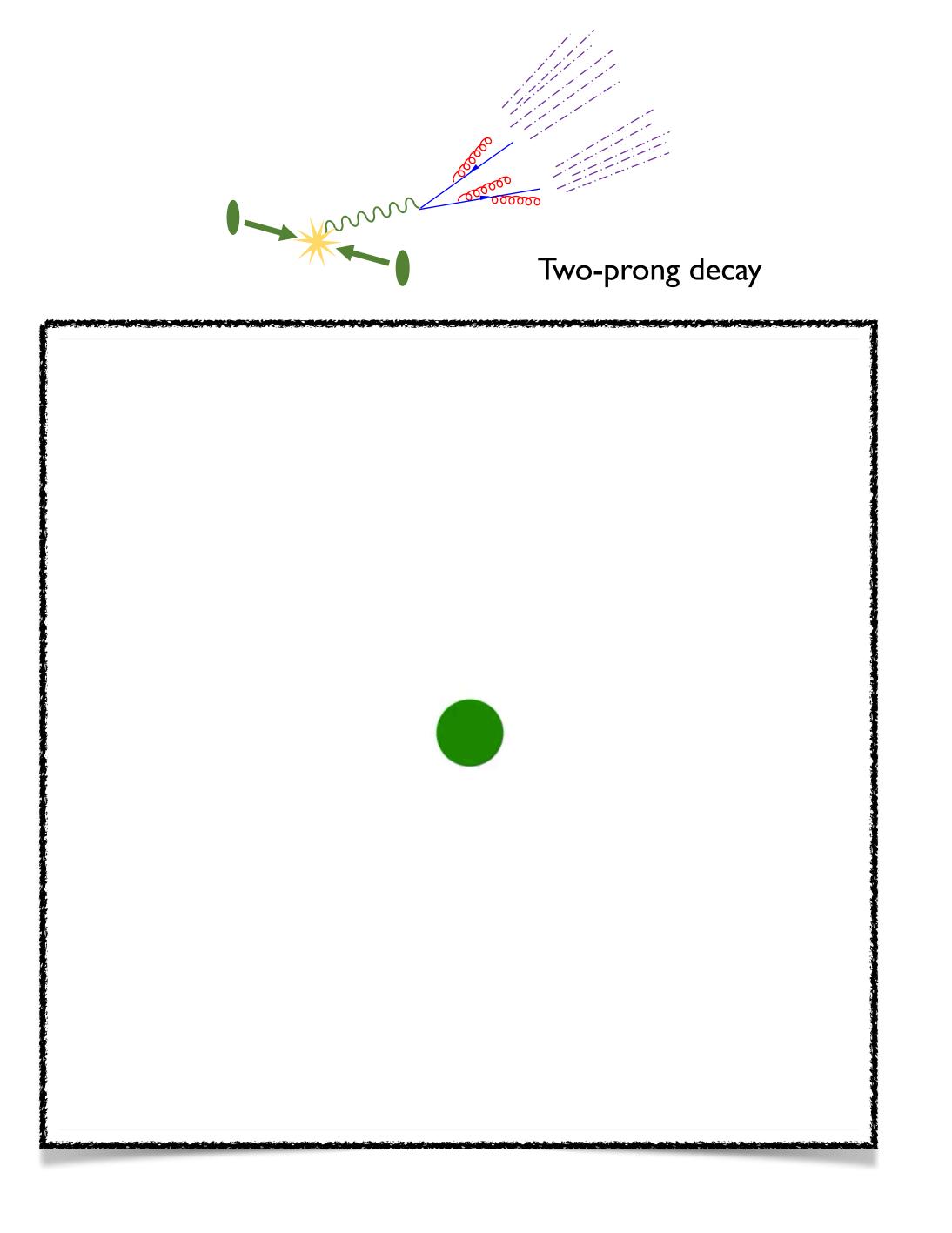
Visualizing Jet Formation – W Jets





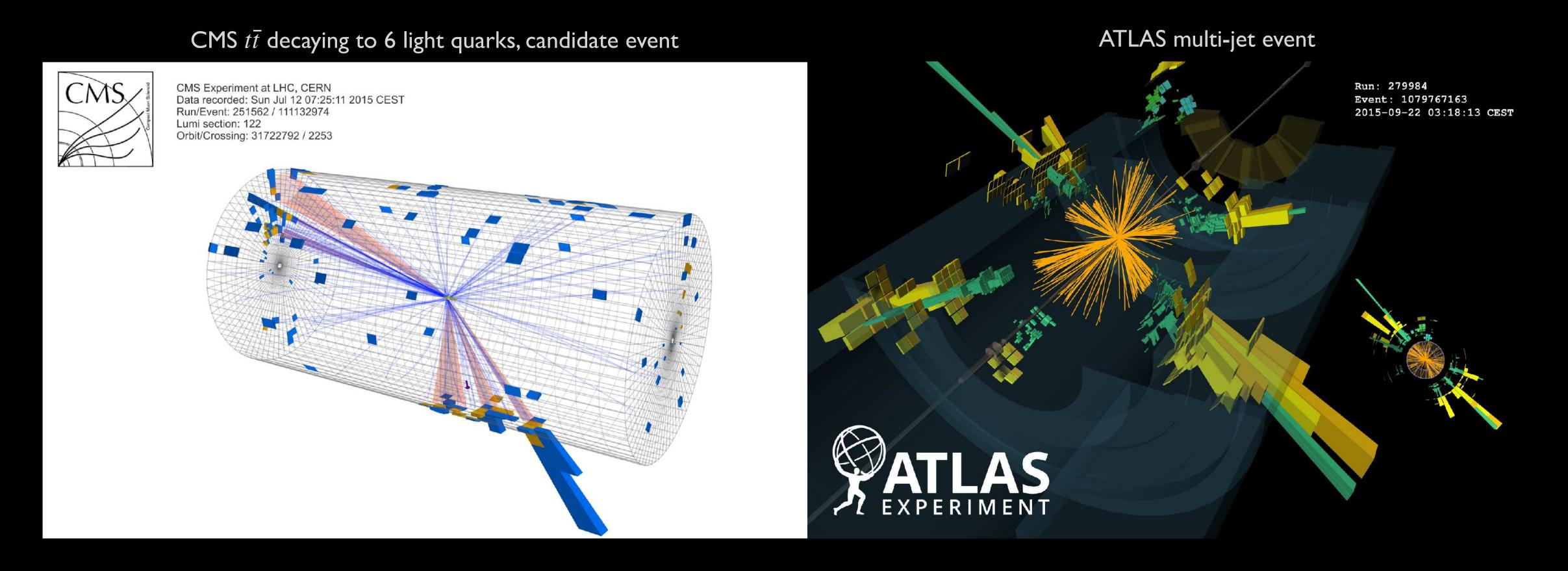
Visualizing Jet Formation – W Jets





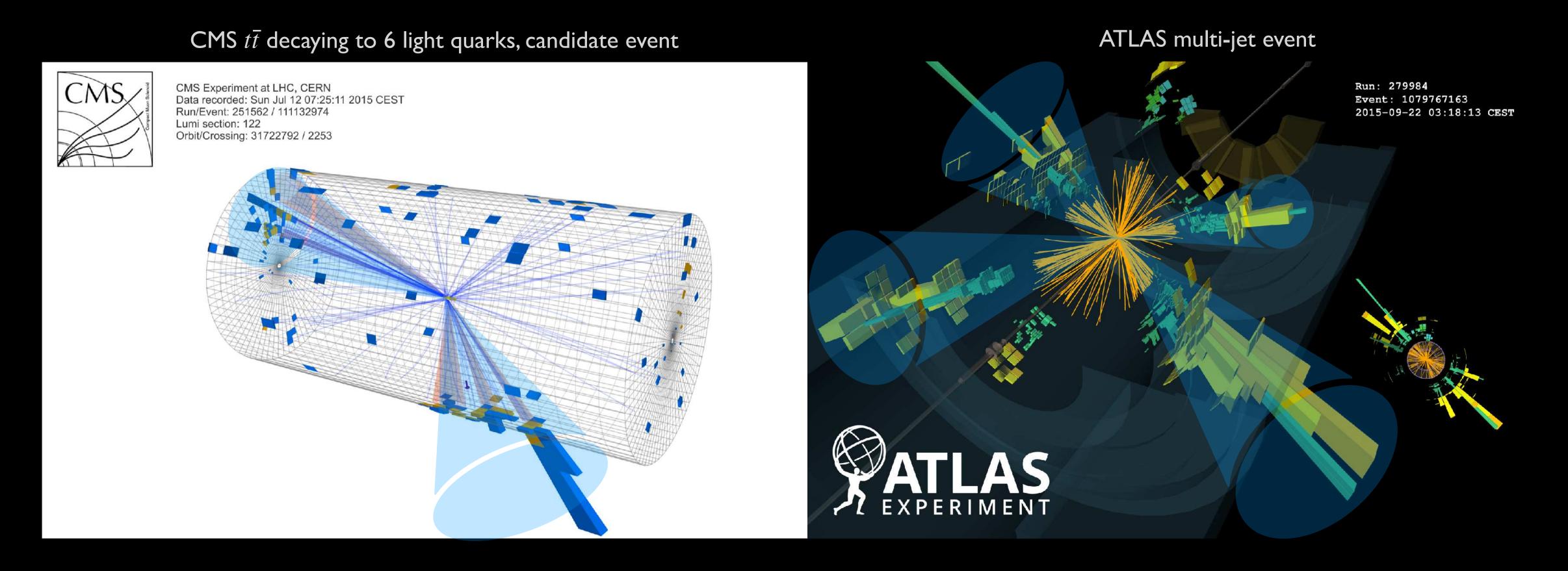
Jet Formation at the LHC

Jets are collimated sprays of particles arising from production of high-energy quarks and gluons



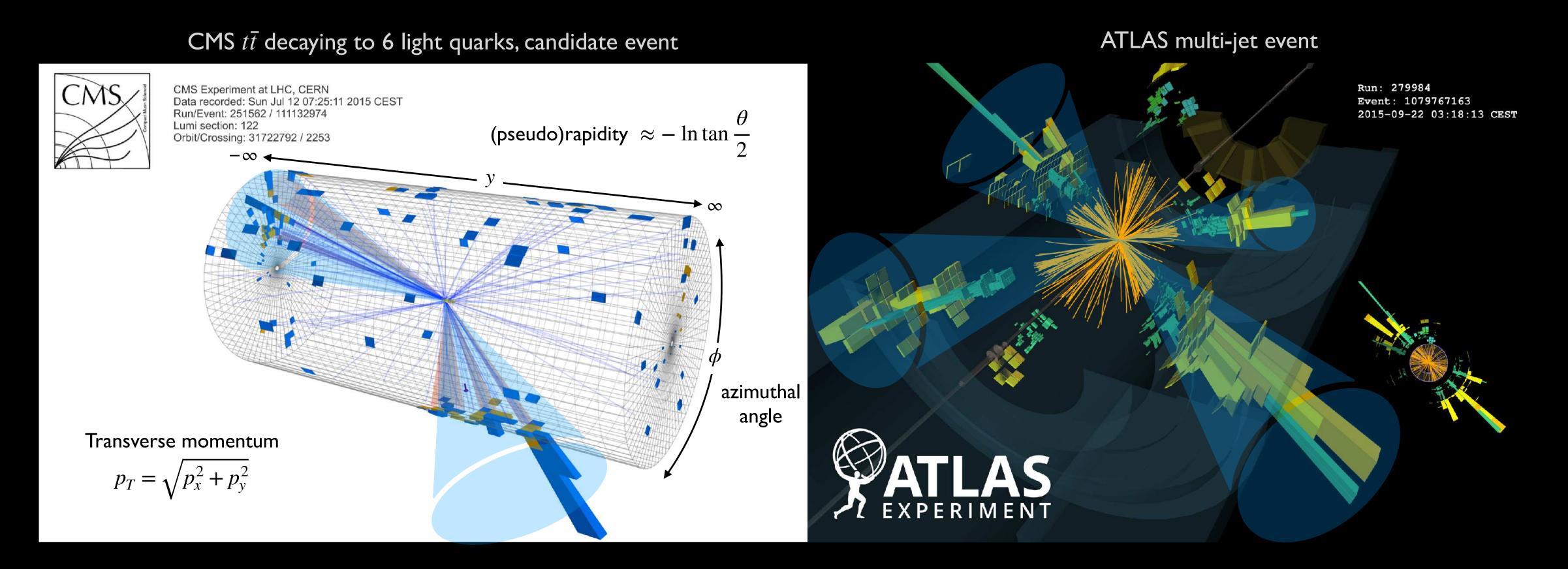
Jet Formation at the LHC

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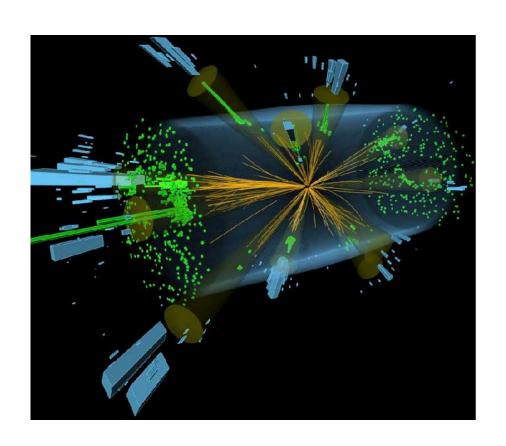


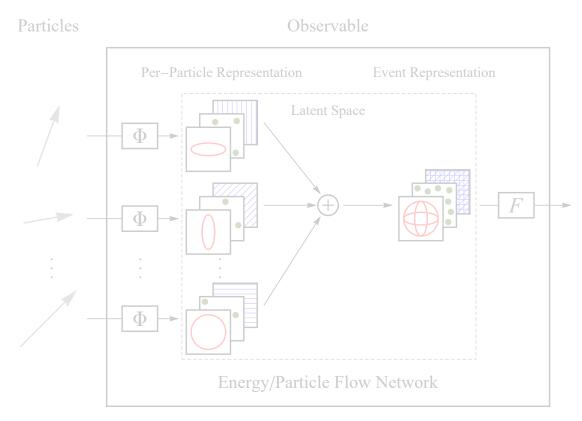
Jet Formation at the LHC

Jets are collimated sprays of particles arising from production of high-energy quarks and gluons



Jets are defined via sequential recombination of particles (hierarchical agglomerative clustering)





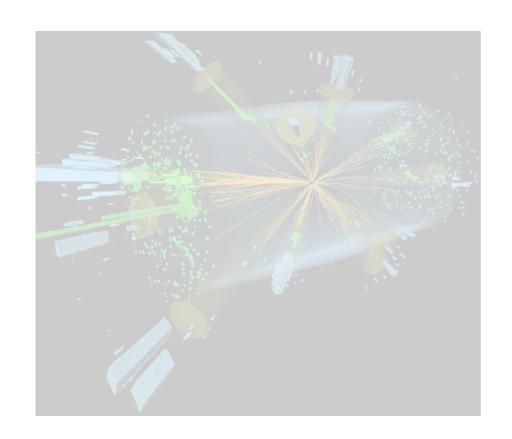


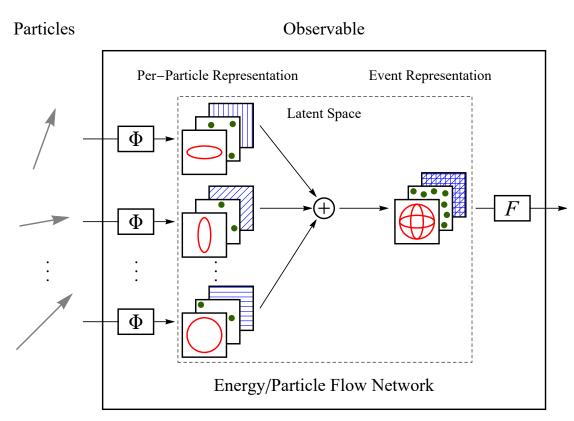
Particle Physics Fundamentals – Jets

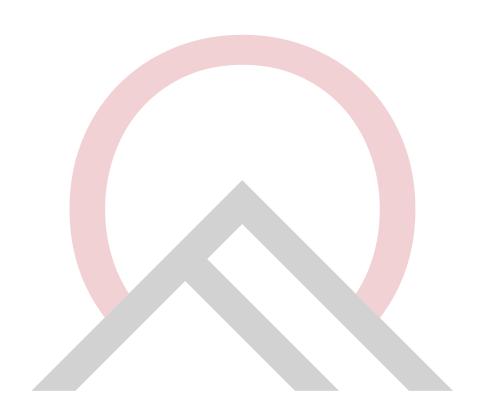
Jets are critical to the success of the modern collider program

Architectures for Colliders

Statistical Deconvolution







Particle Physics Fundamentals – Jets

Jets are critical to the success of the modern collider program

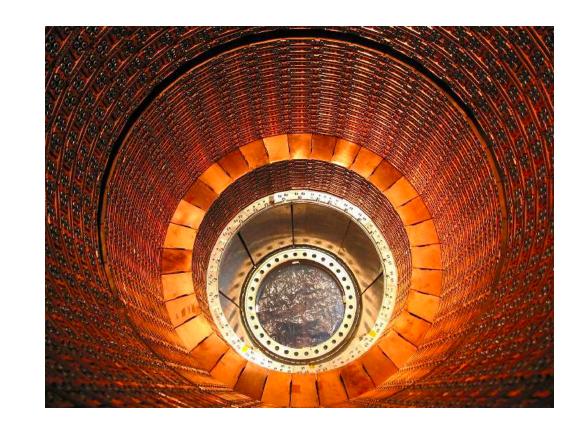
Architectures for Colliders

How do we build a neural network architecture for collider events?

Statistical Deconvolution

Representing Jets as Images

[Cogan, Kagan, Strauss, Schwartzman, JHEP 2015; de Oliviera, Kagan, Mackey, Nachman, Schwartzman, JHEP 2016; PTK, Metodiev, Schwartz, JHEP 2017]



as

Take advantage of existing tools for processing images

Pixel intensities ~ transverse momenta of calorimeter cell

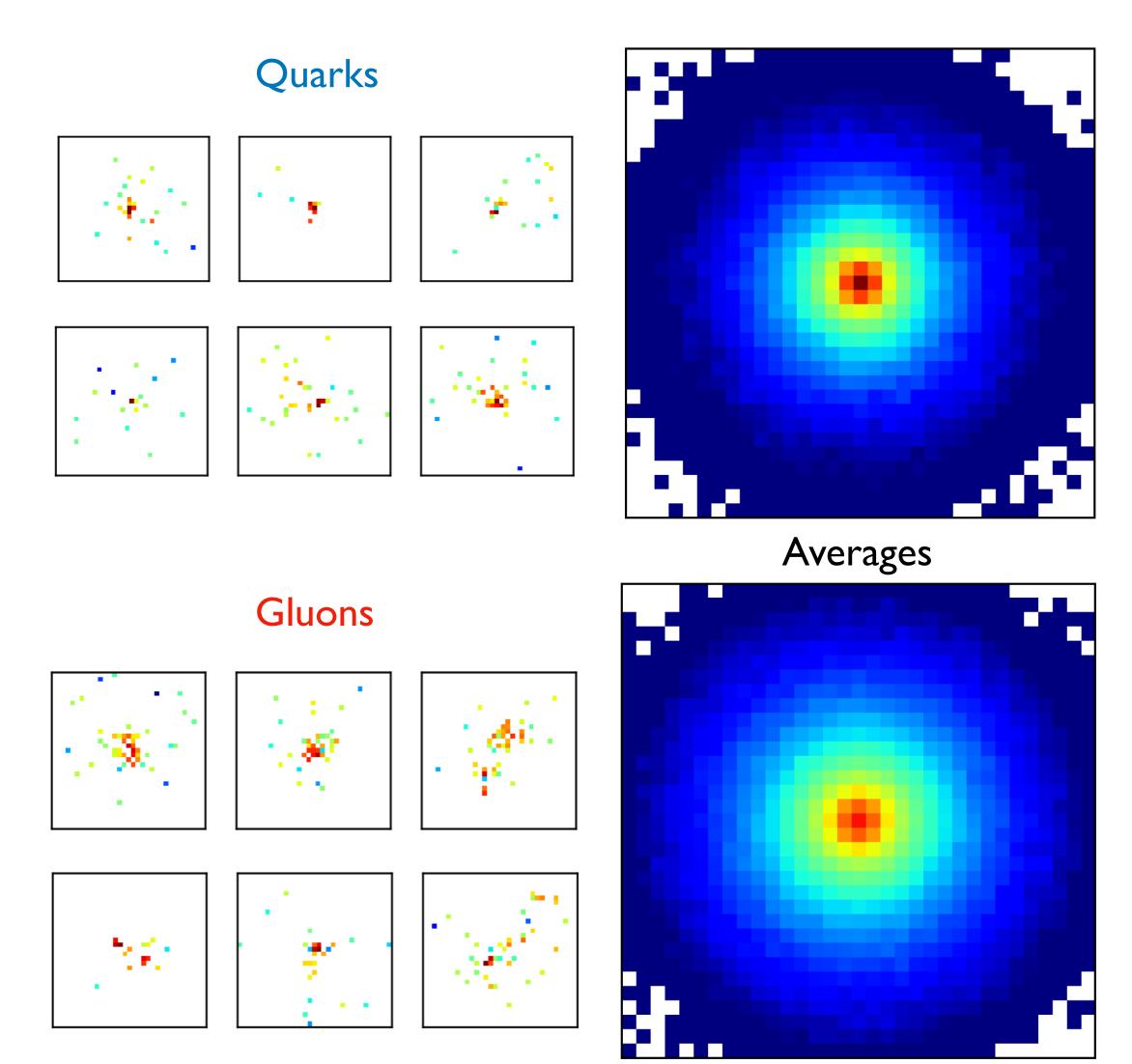
Center on patch of rapidity-azimuth $(y - \phi)$ plane containing a jet

"Color" (i.e. multiple channel) images possible, e.g.:

Red: p_T of charged particles

Green: p_T of neutral particles

Blue: charged particle multiplicity

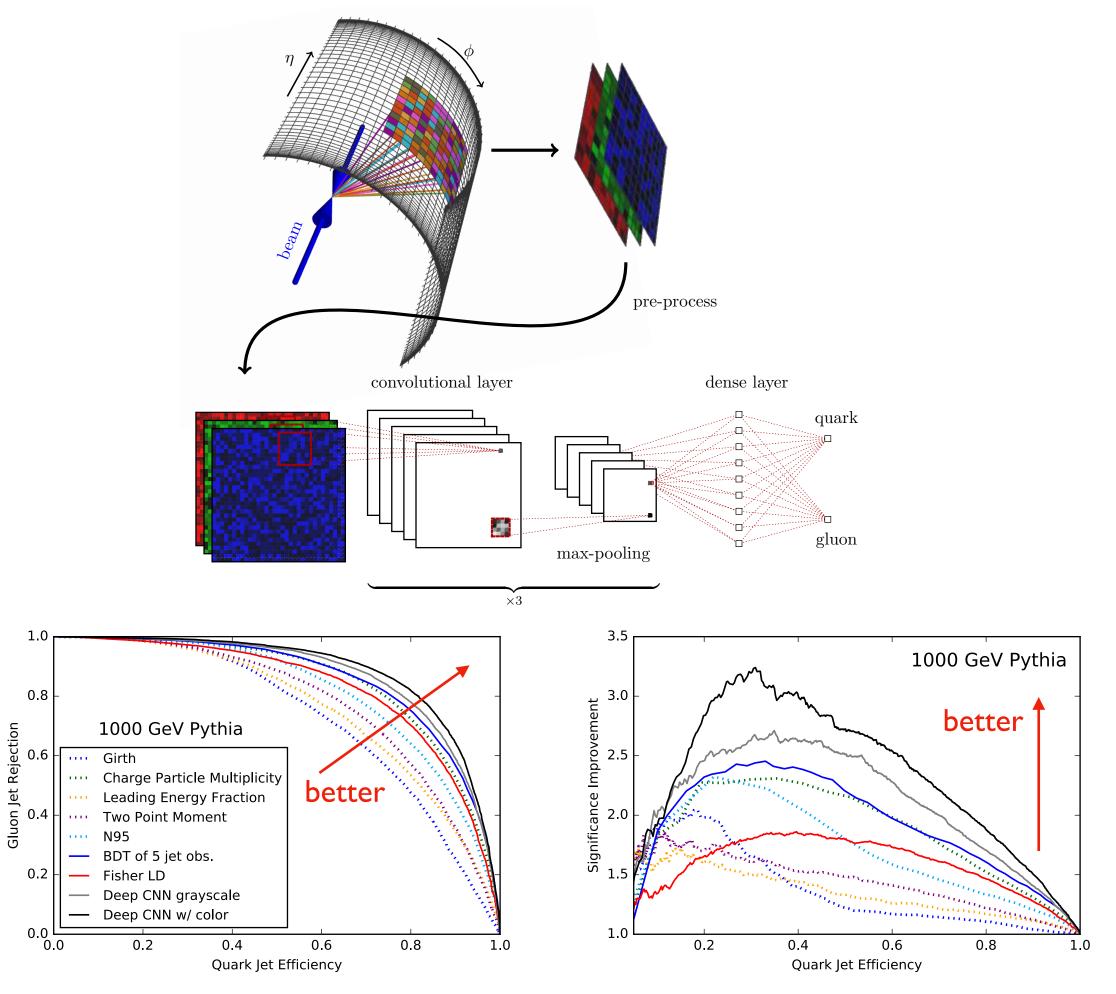


Classification and Regression with Jet Images and Convolutional NNs

Deep Learning in Color

[PTK, Metodiev, Schwartz, JHEP 2017]

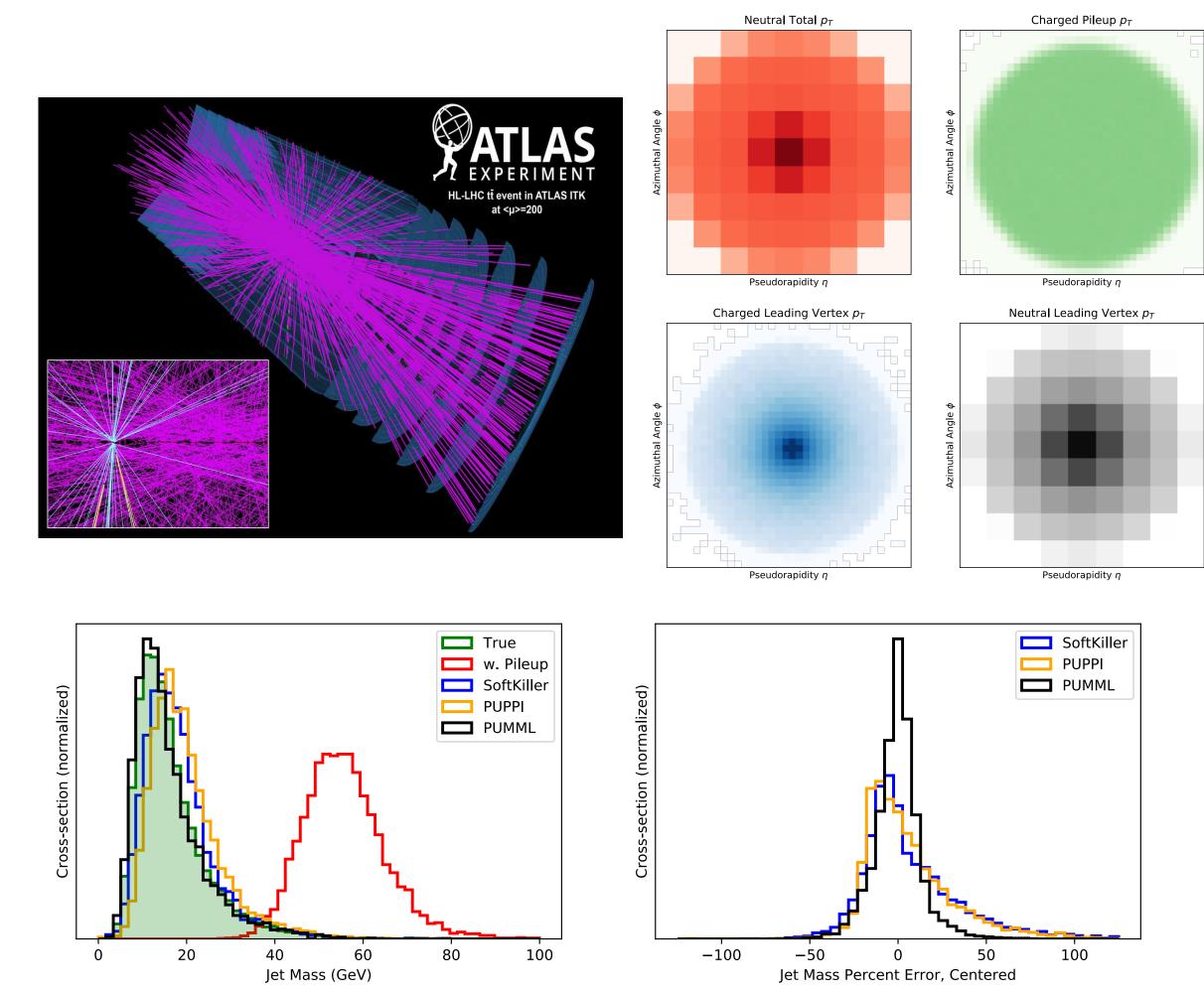
Quark and gluon jet classification with multi-channel jet images



Pileup Mitigation with Machine Learning (PUMML)

[PTK, Metodiev, Nachman, Schwartz, JHEP 2017]

Pileup removal via regression to the "leading vertex" jet image



Better Neural Network Architectures for Particle Physics

Maximally appropriate ML architectures respect symmetries of the underlying data

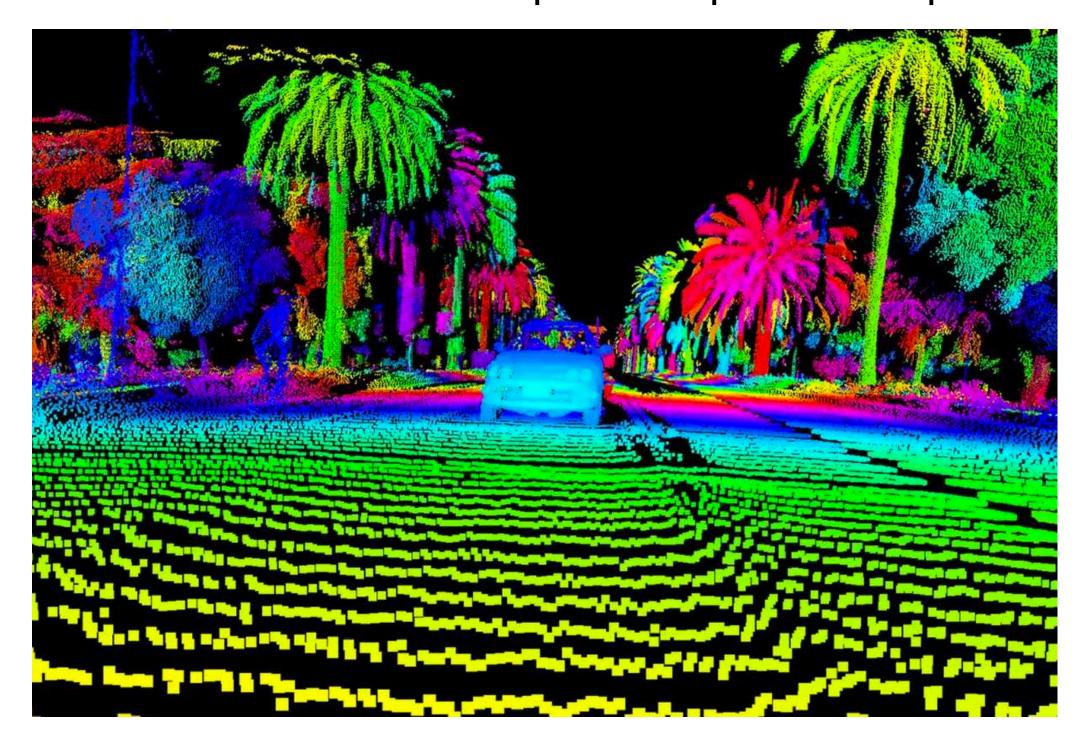
Particle physics events are naturally "point clouds"

Better Neural Network Architectures for Particle Physics

Maximally appropriate ML architectures respect symmetries of the underlying data

Particle physics events are naturally "point clouds"

Point cloud: "A set of data points in space" – Wikipedia



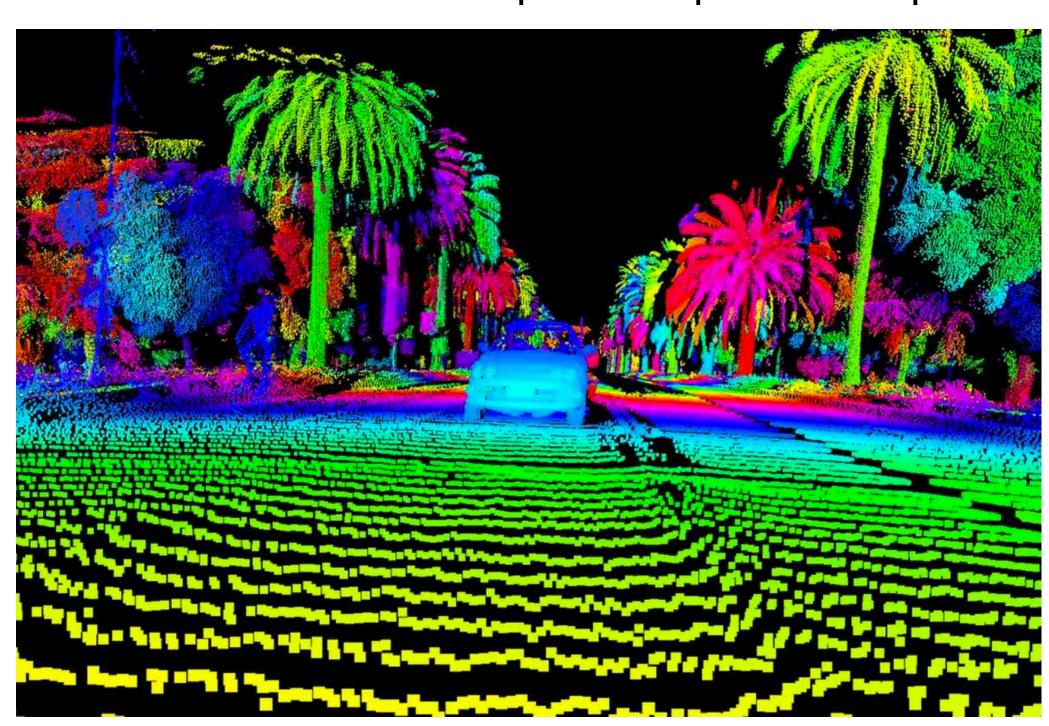
LIDAR data from self-driving car sensor

Better Neural Network Architectures for Particle Physics

Maximally appropriate ML architectures respect symmetries of the underlying data

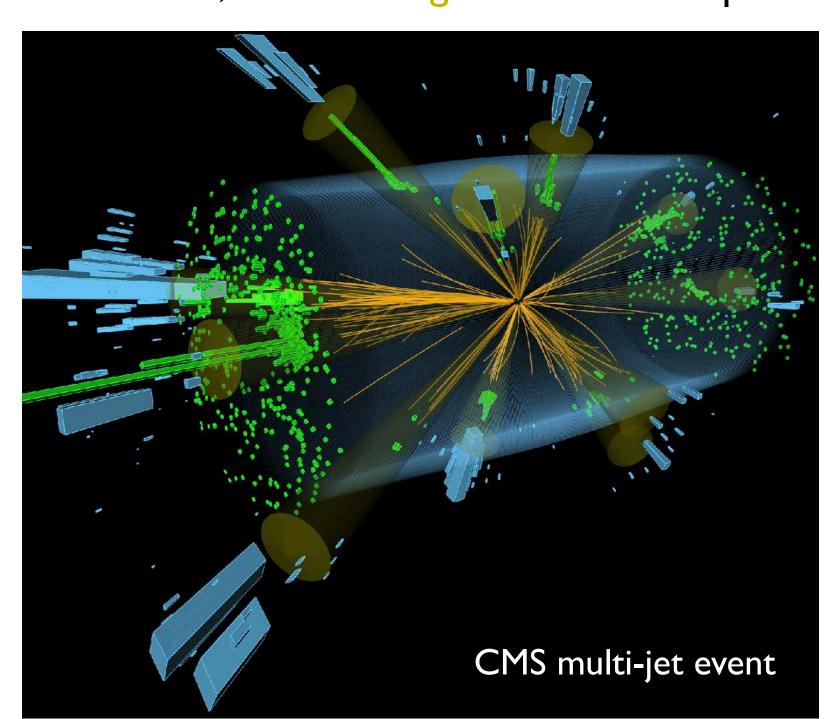
Particle physics events are naturally "point clouds"

Point cloud: "A set of data points in space" – Wikipedia



LIDAR data from self-driving car sensor

An unordered, variable length collection of particles



particle $\in \mathbb{R}^d$ $\{p_T, y, \phi, \ldots\}$

event $\in \mathbb{R}^{M \times d}$

Due to quantum-mechanical indistinguishability

Due to probabilistic nature of event formation

Deep Sets for Particle Jets

[Zaheer, Kottur, Ravanbhakhsh, Póczos, Salakhutdinov, Smola, NeurIPS 2017; PTK, Metodiev, Thaler, JHEP 2019]

Provable decompositions of symmetric functions

(See backup for details)

Energy Flow Network (EFN)

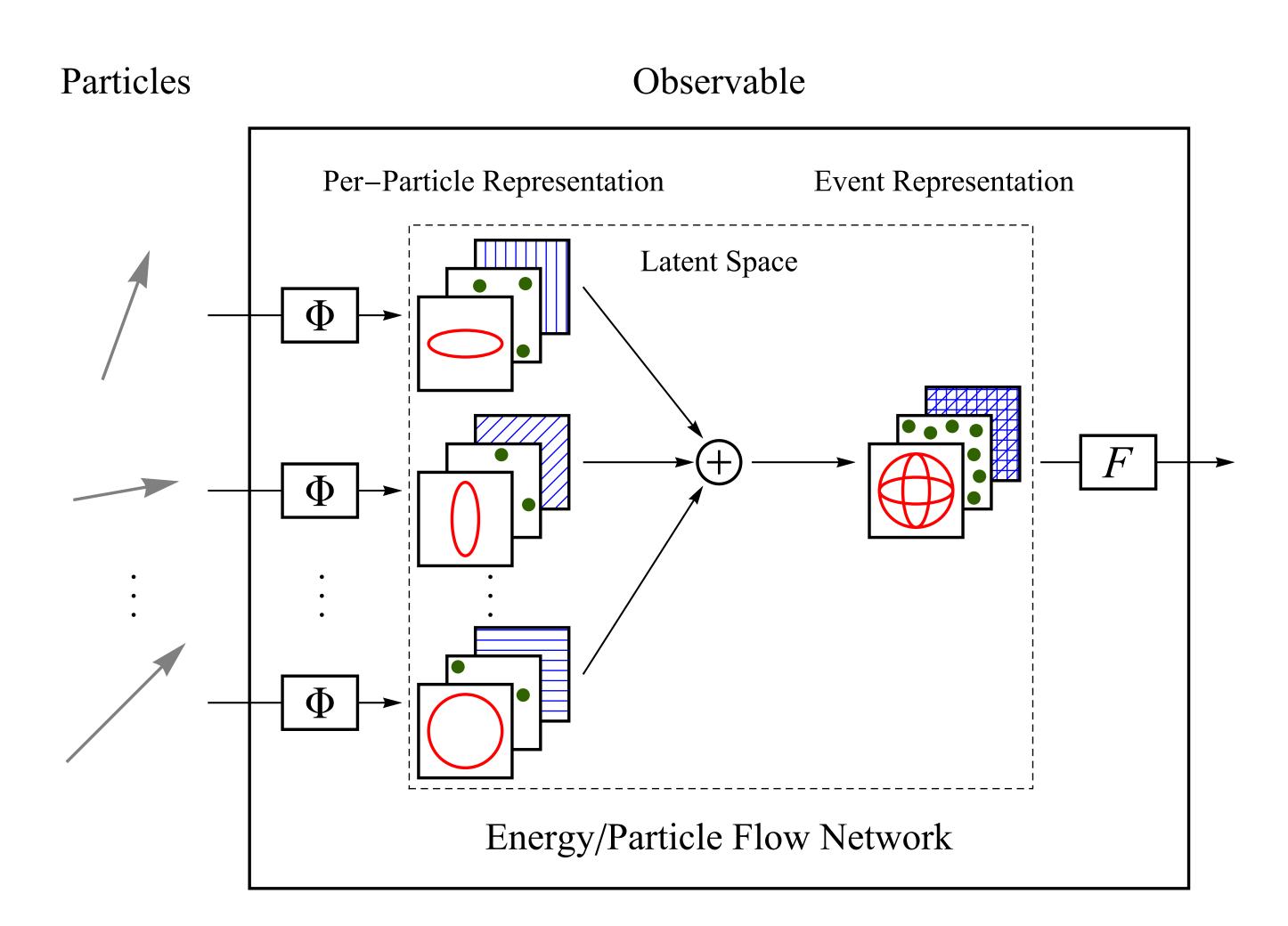
$$EFN(\{p_1^{\mu}, \dots, p_M^{\mu}\}) = F\left(\sum_{i=1}^{M} z_i \Phi(\hat{p}_i)\right)$$

Energy-weighted (IRC-safe) latent space

Particle Flow Network (PFN)

$$PFN(\{p_1^{\mu}, \dots, p_M^{\mu}\}) = F\left(\sum_{i=1}^{M} \Phi(p_i^{\mu})\right)$$

Fully general latent space



EnergyFlow Python package contains EFN and PFN implementations in Tensorflow

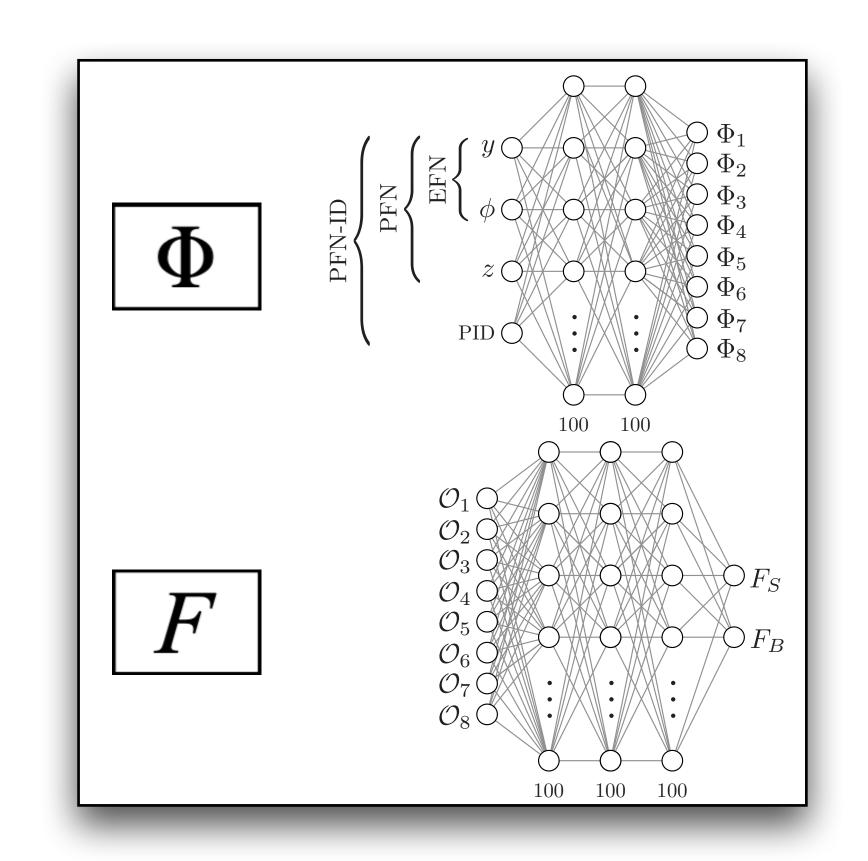
Approximating Φ and F with Neural Networks

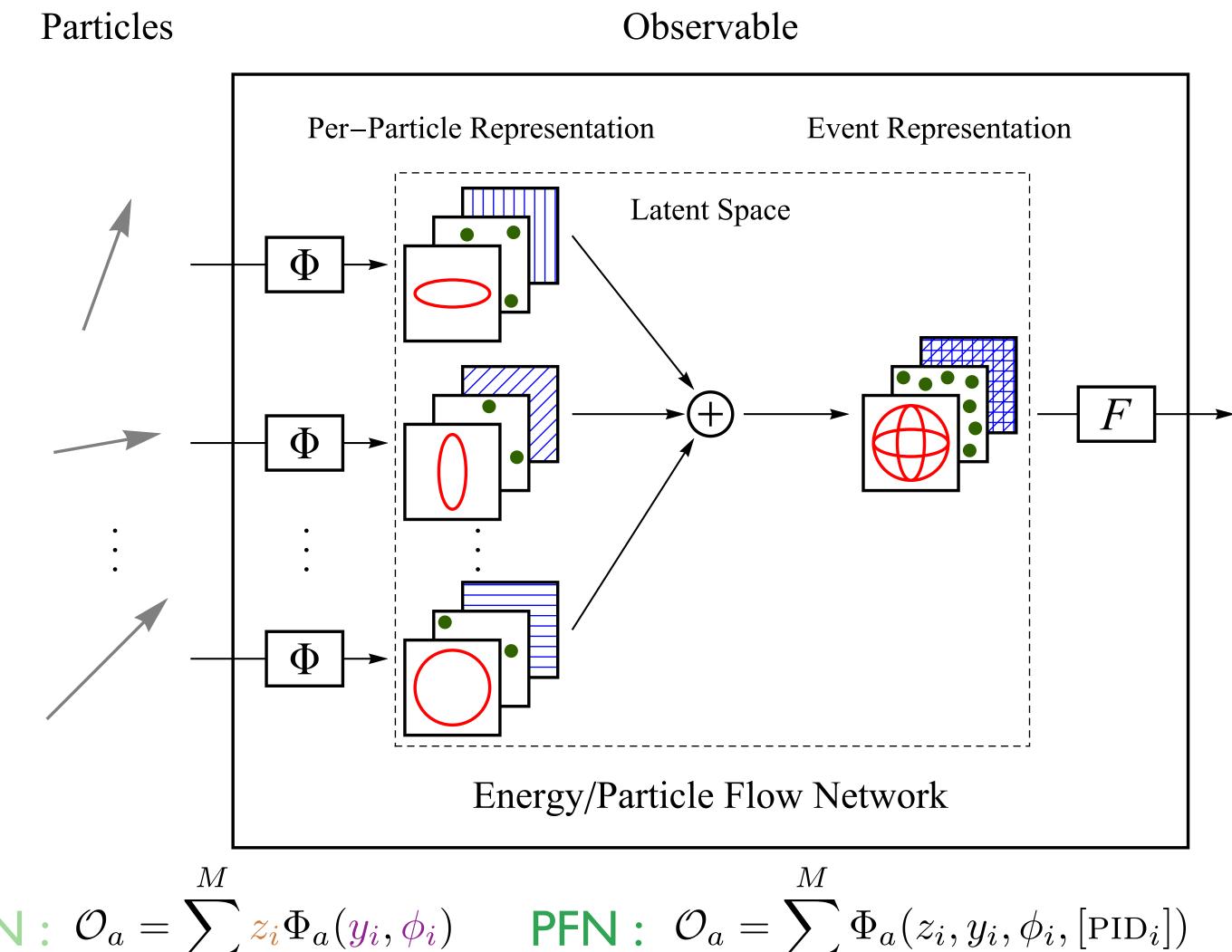
[PTK, Metodiev, Thaler, JHEP 2019]

Employ neural networks as arbitrary function approximators

Use fully-connected networks for simplicity

Default sizes $-\Phi$: (100, 100, ℓ), F: (100, 100, 100)





$$\mathsf{EFN}: \ \mathcal{O}_a = \sum_{i=1}^M z_i \Phi_a(y_i, \phi_i) \qquad \mathsf{PFN}: \ \mathcal{O}_a = \sum_{i=1}^M \Phi_a(z_i, y_i, \phi_i, [\mathtt{PID}_i])$$

Quark vs. Gluon: Latent Dimension Sweep

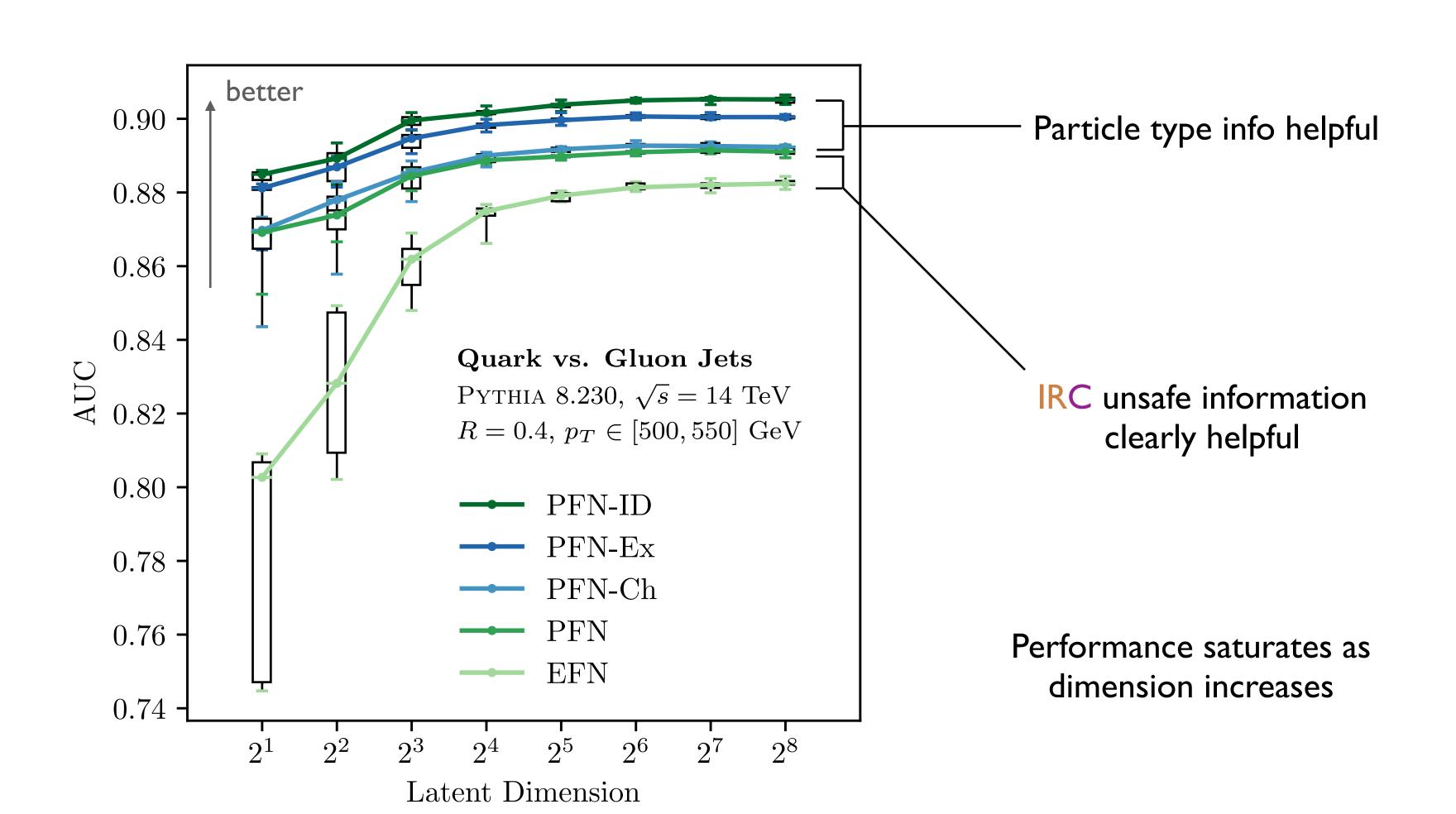
PFN-ID: Full particle flavor info $(\gamma, \pi^{\pm}, K^{\pm}, K_L, p, \bar{p}, n, \bar{n}, e^{\pm}, \mu^{\pm})$

PFN-Ex: Experimentally accessible info $(\gamma, h^{\pm,0}, e^{\pm}, \mu^{\pm})$

PFN-Ch: Particle charge info (+,0,-)

PFN: No particle type info, arbitrary energy dependence

EFN: IRC-safe latent space



Quark vs. Gluon: Classification Performance

[PTK, Metodiev, Thaler, JHEP 2019]

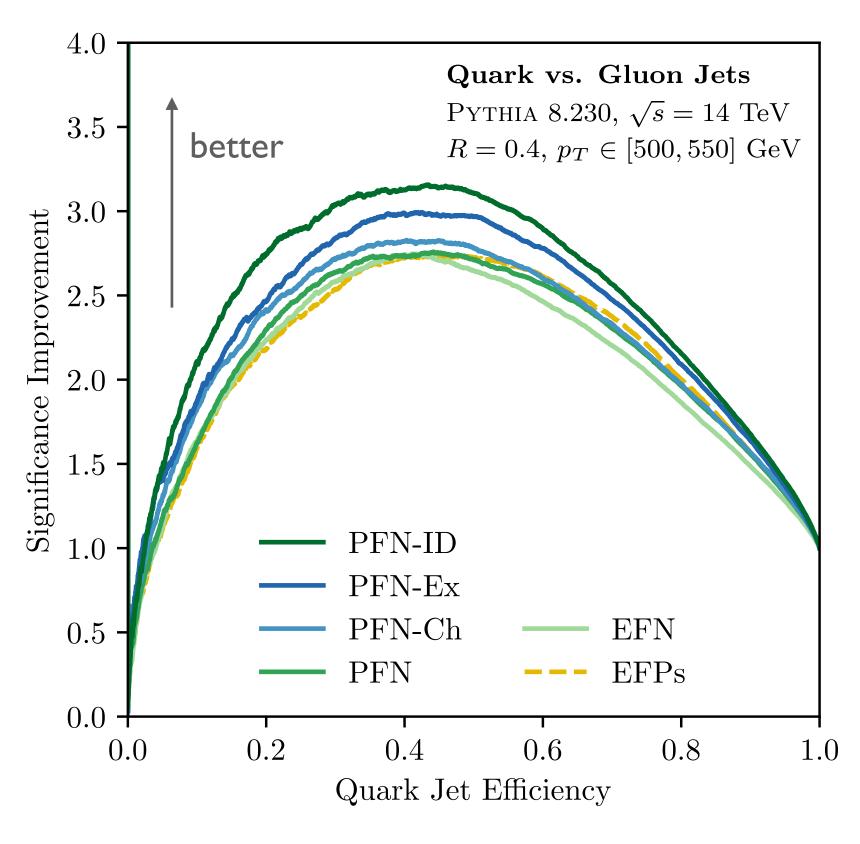
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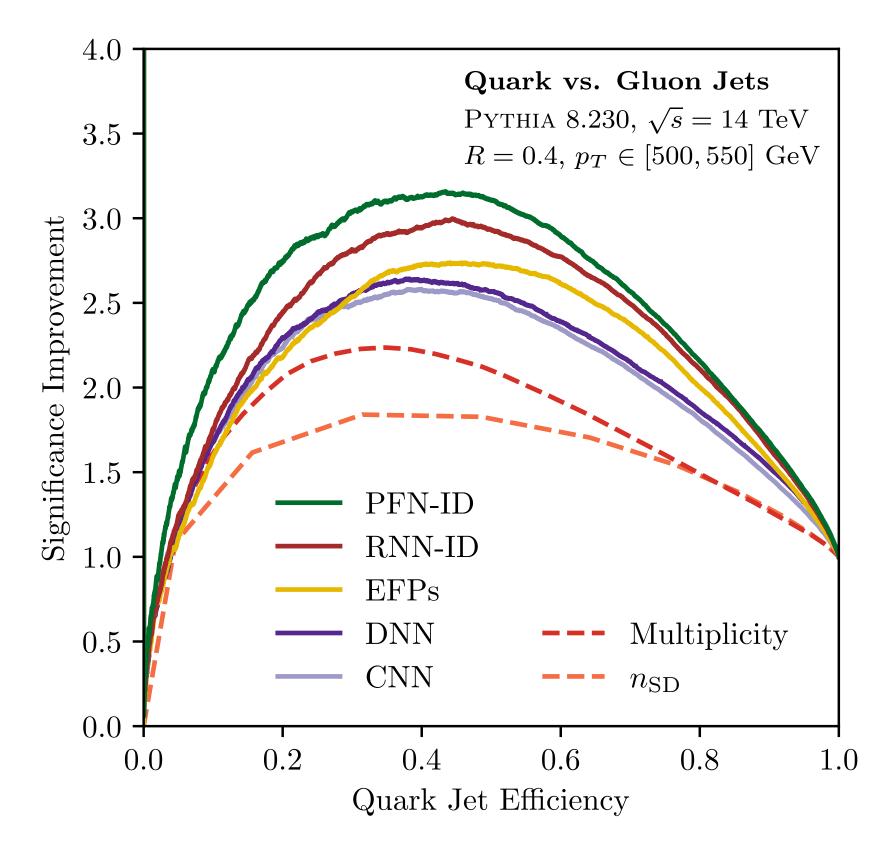
PFN: No particle type info, arbitrary energy dependence

EFN: IRC-safe latent space



Latent space dimension $\ell = 256$

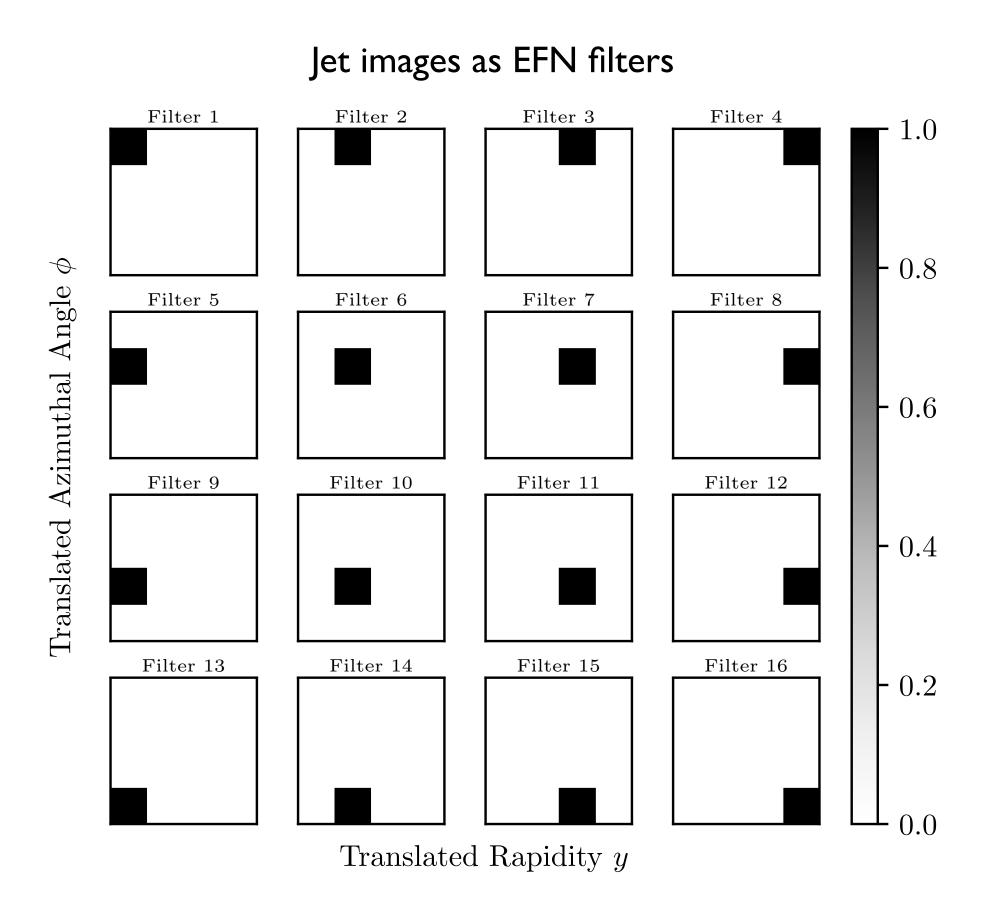
EFPs are comparable to EFN

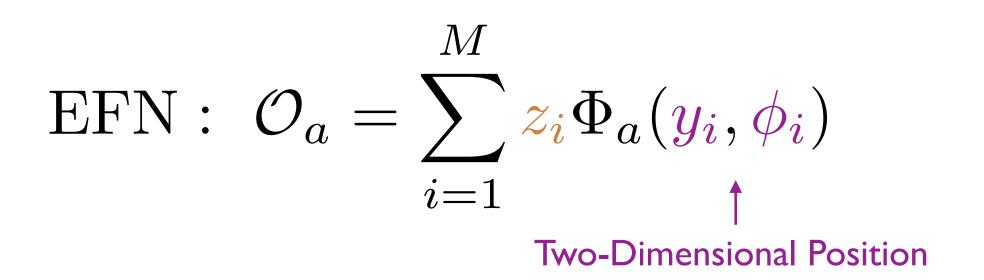


PFN-ID better than RNN-ID

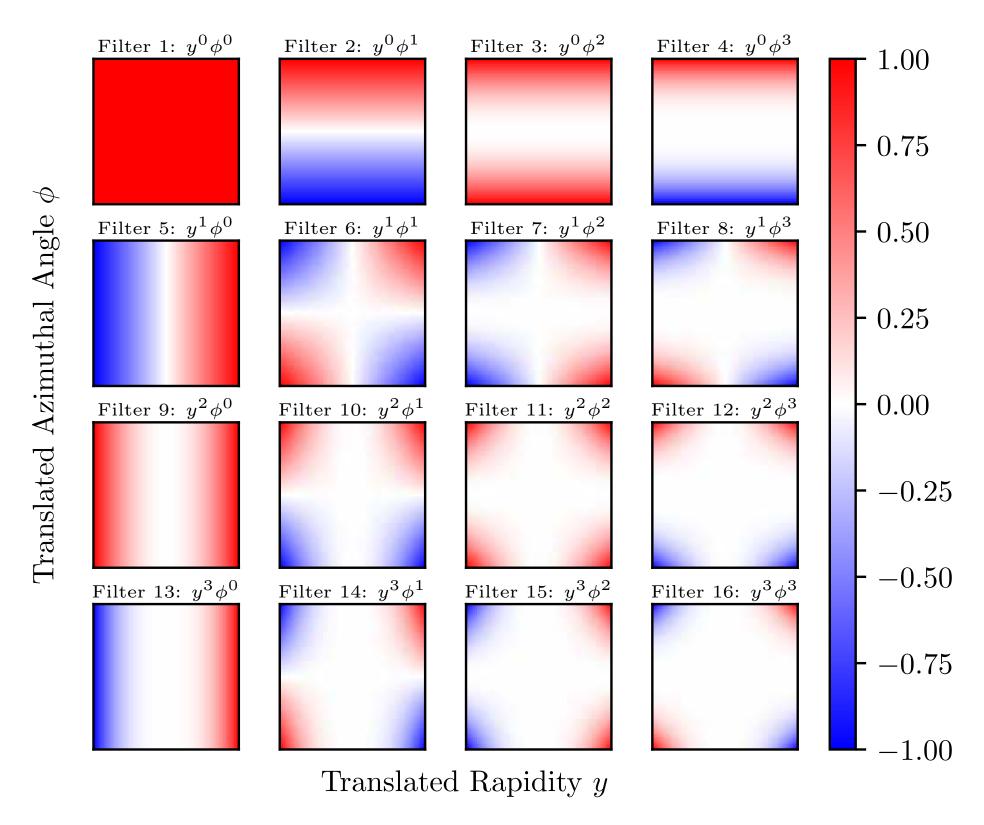
Energy Flow Network Visualization

Visualize EFN observables as 2D filters in the translated rapidity-azimuth plane





Moments as EFN filters

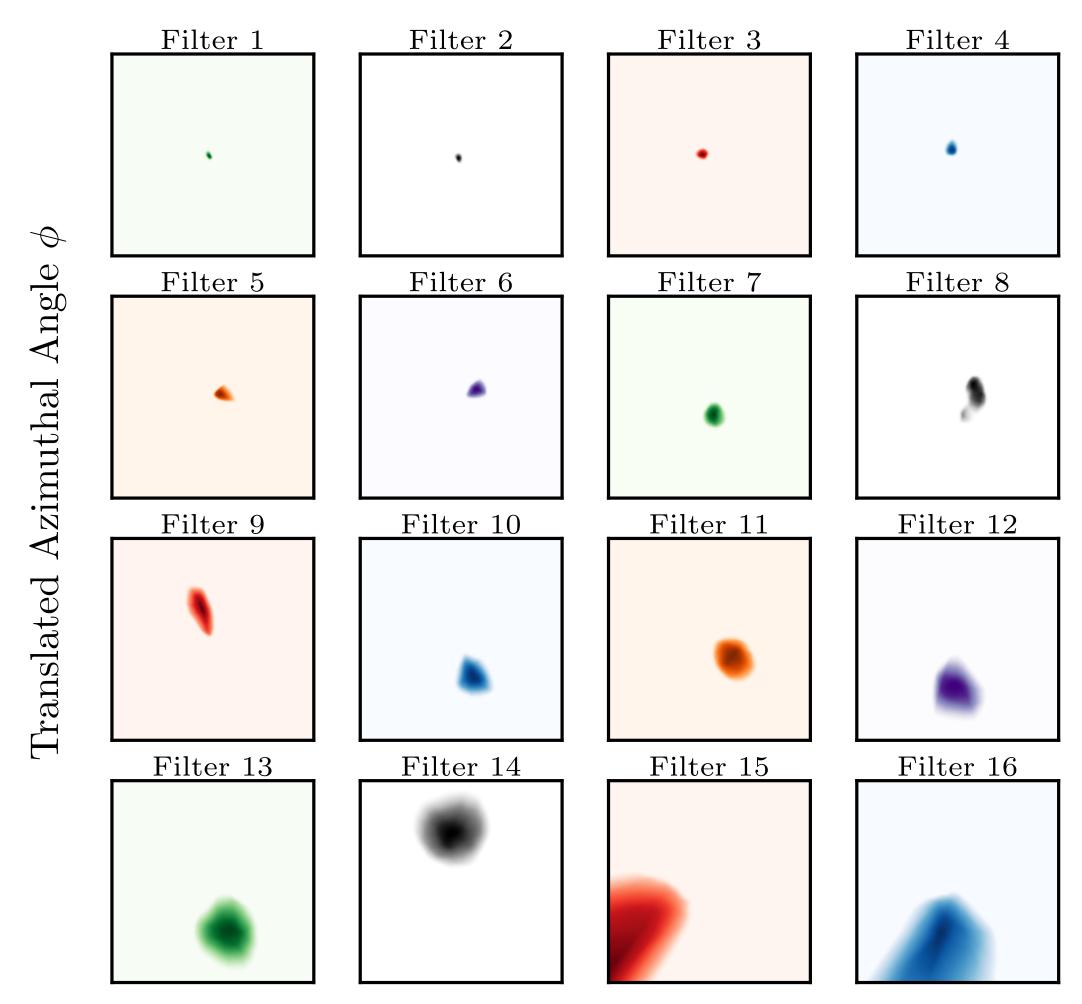


[Donoghue, Low, Pi, <u>PRD 1979</u>; Gur-Ari, Papucci, Perez, <u>1101.2905</u>; PTK, Metodiev, Thaler, <u>PRD 2020</u>]

Energy Flow Network Visualization – Quark vs. Gluon

EFN (ℓ = 256) randomly selected filters, sorted by size

[PTK, Metodiev, Thaler, JHEP 2019]



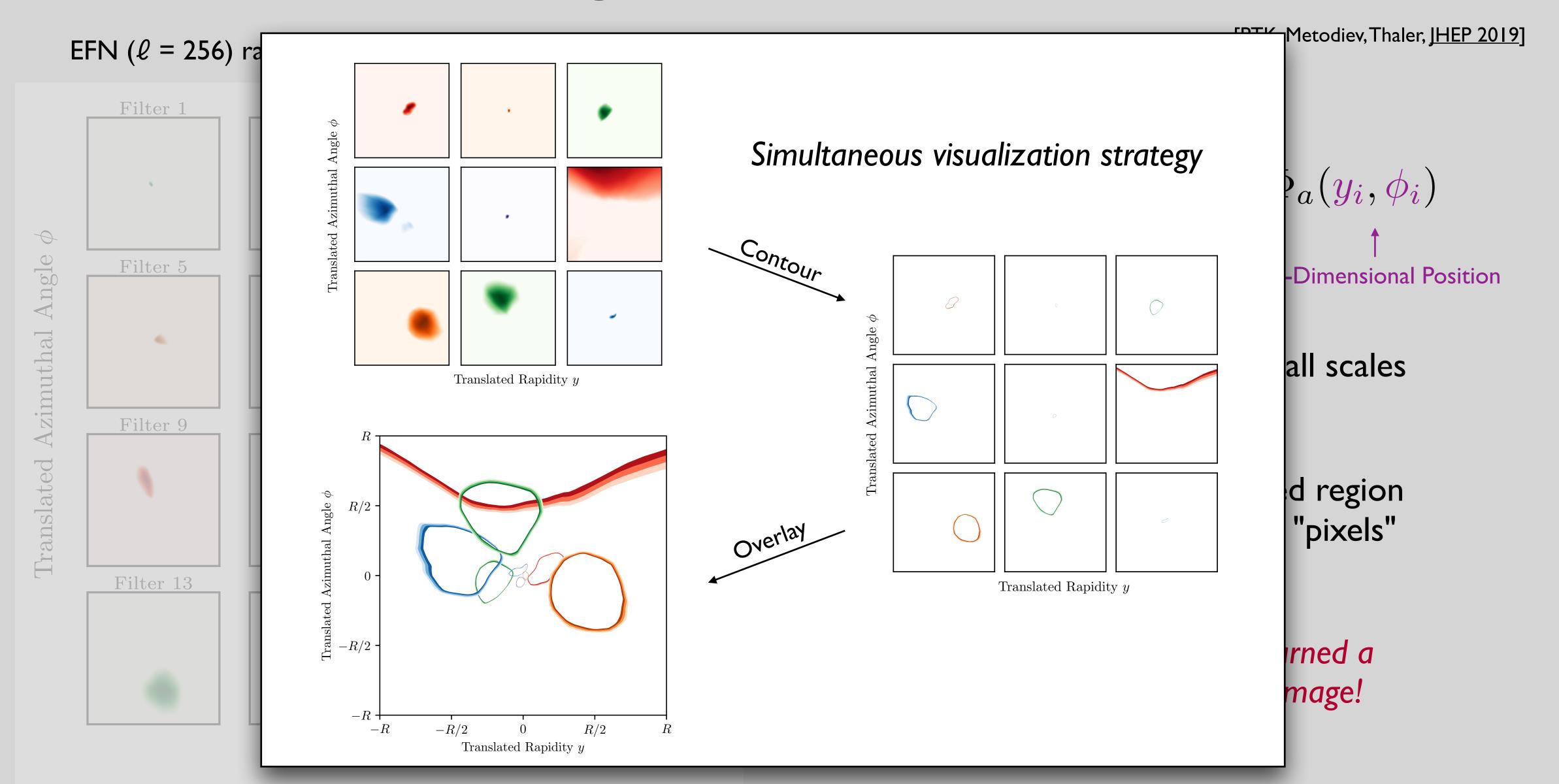
Translated Rapidity y

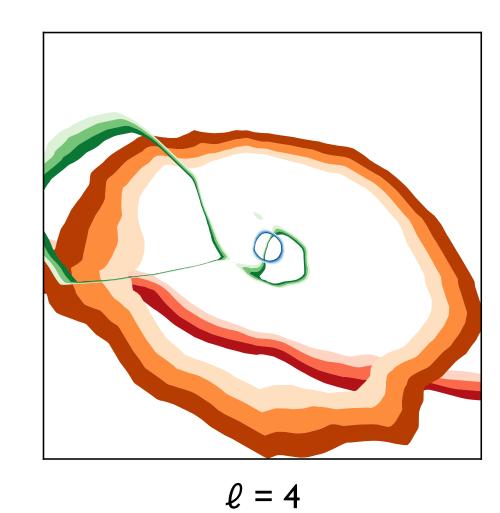
$$ext{EFN}: \ \mathcal{O}_a = \sum_{i=1}^{M} z_i \Phi_a(y_i, \phi_i)$$
 $ext{Two-Dimensional Position}$

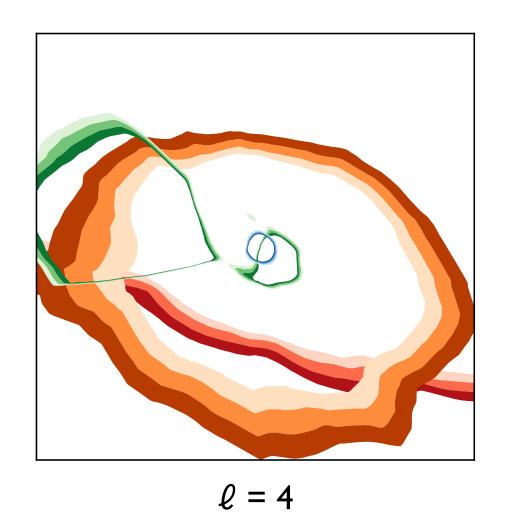
Generally find blobs of all scales

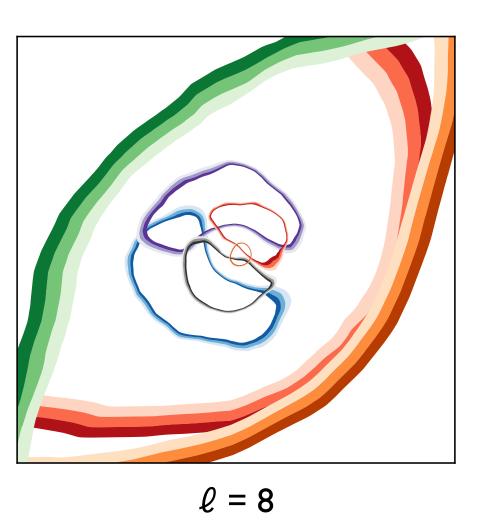
Local nature of activated region lends interpretation as "pixels"

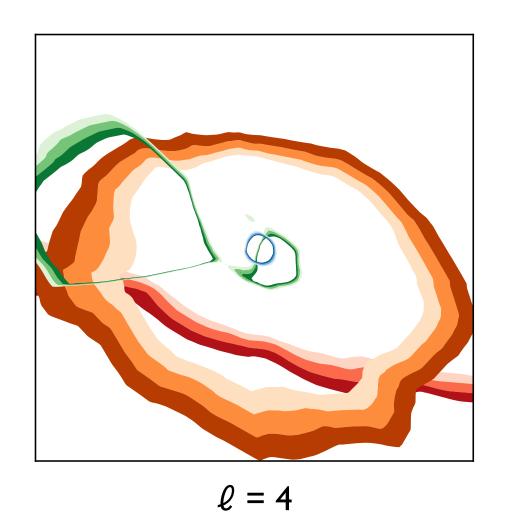
EFN seems to have learned a dynamically sized jet image!

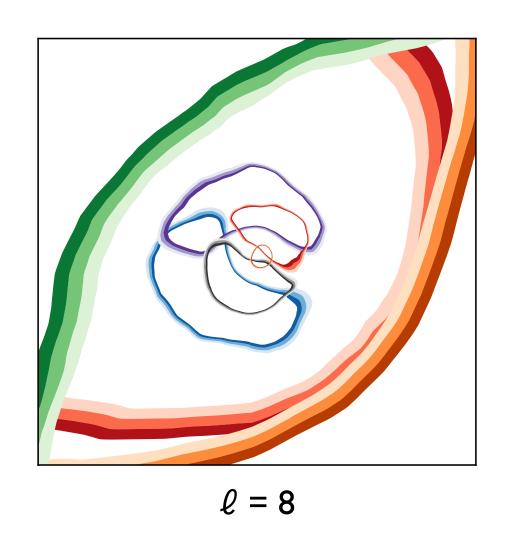


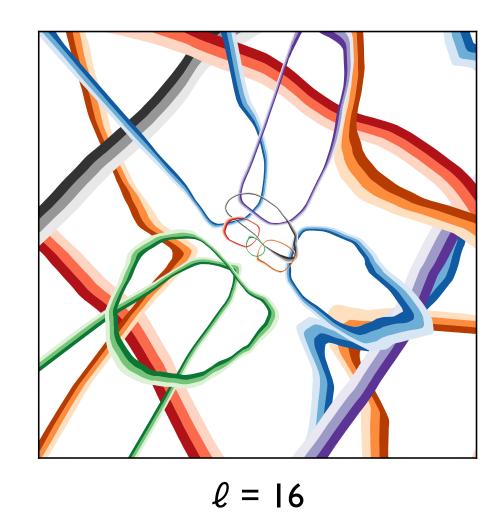


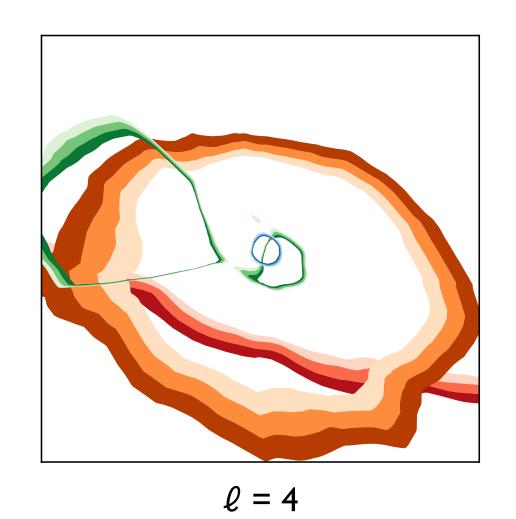


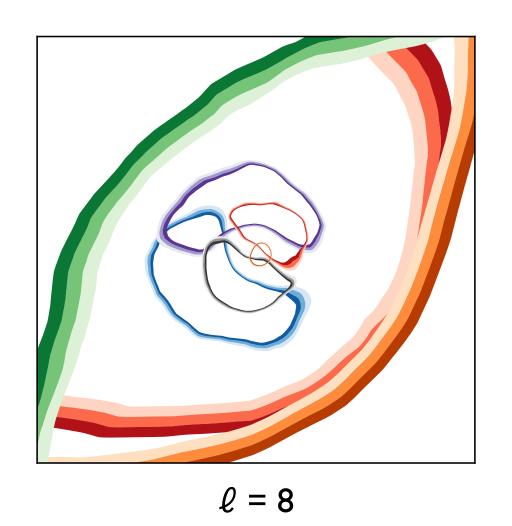


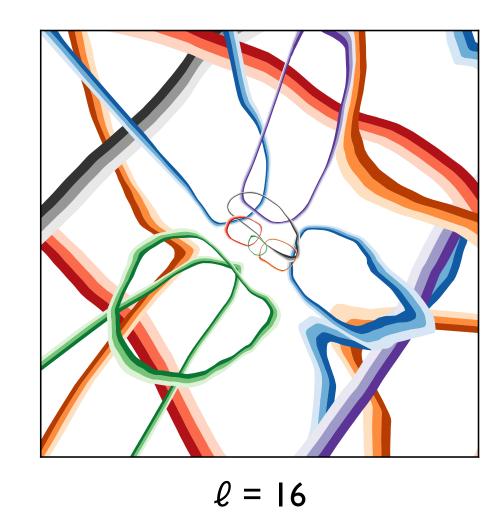


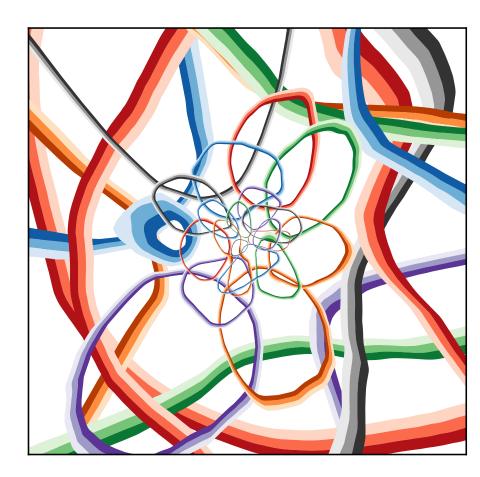


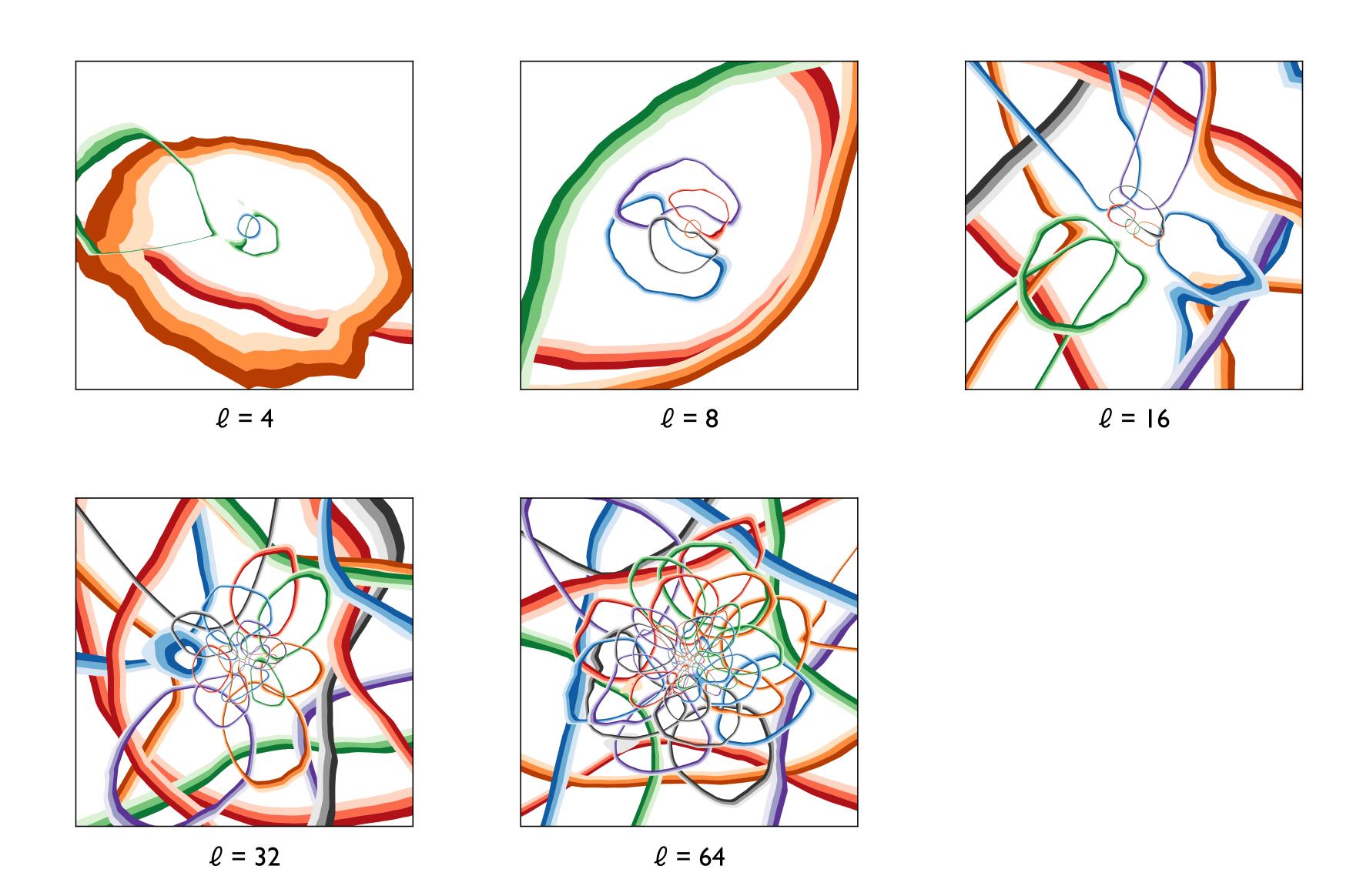


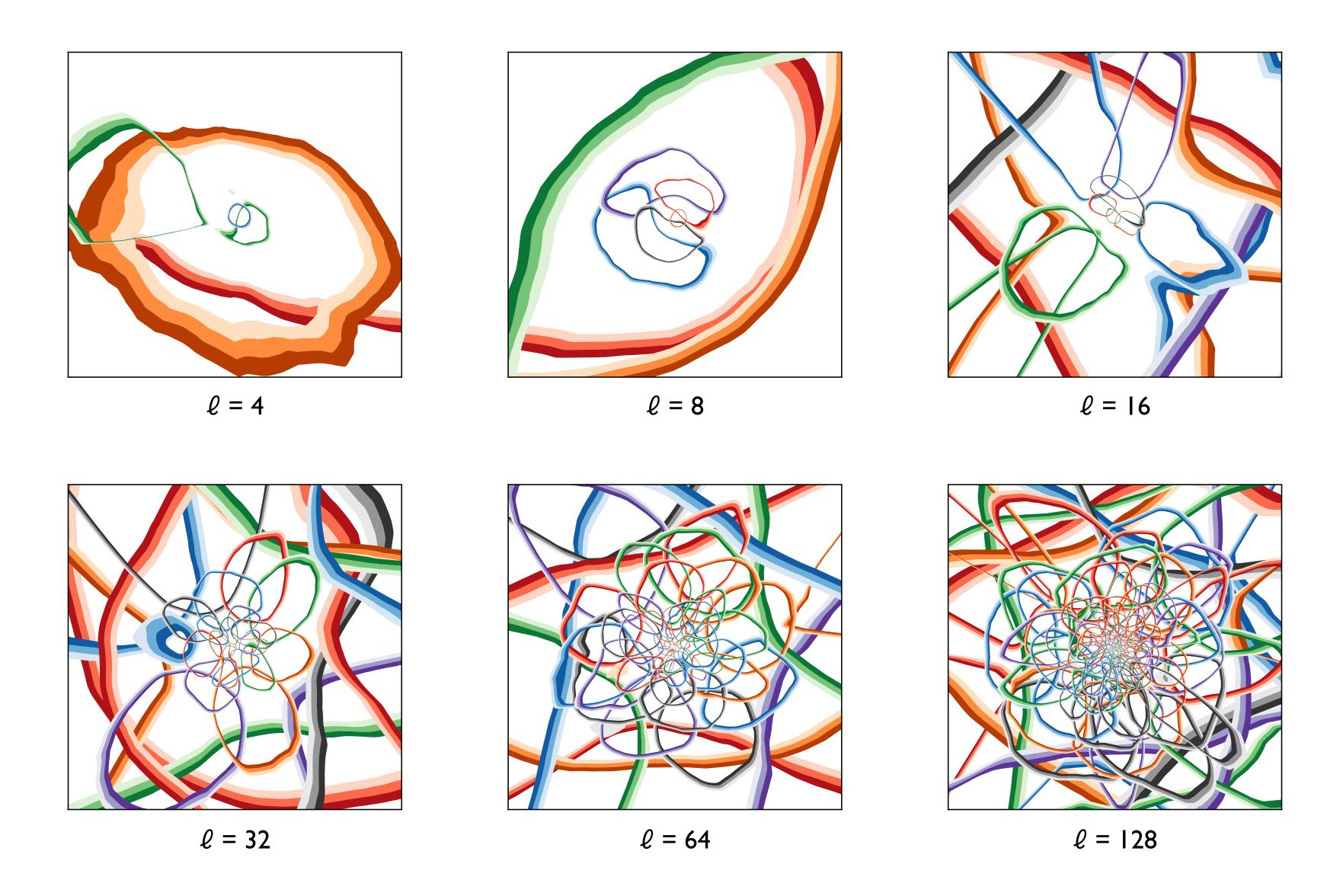


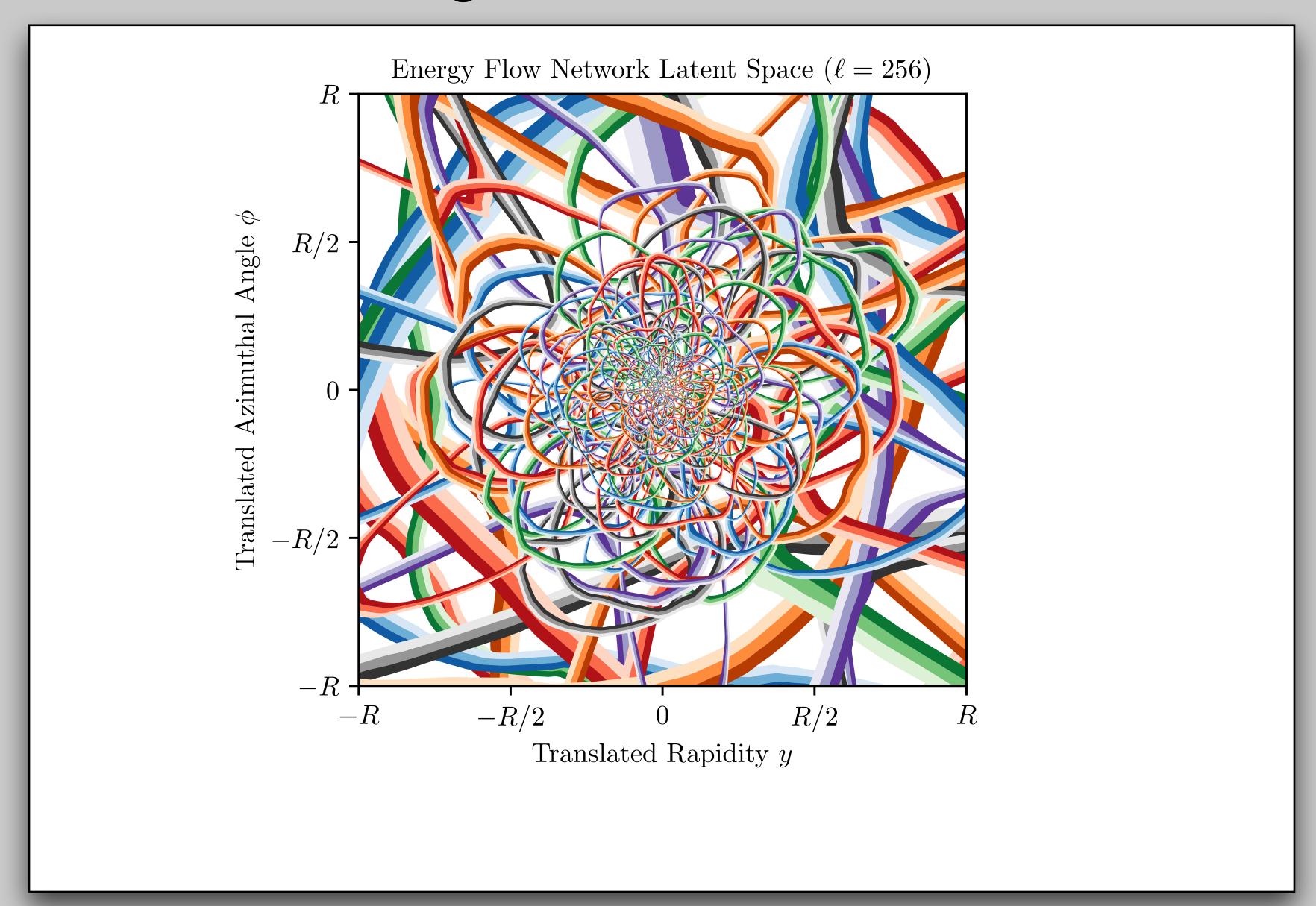


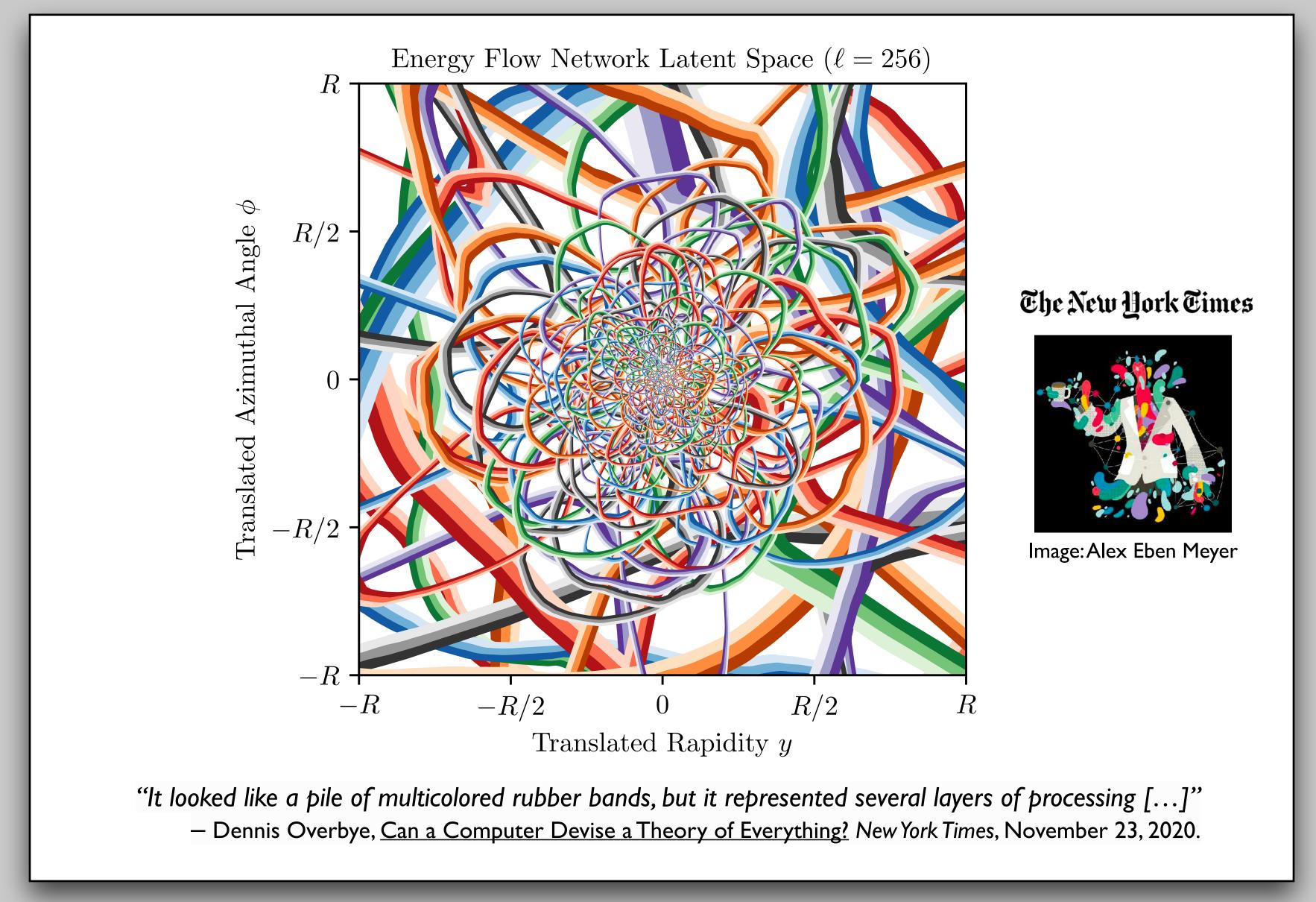






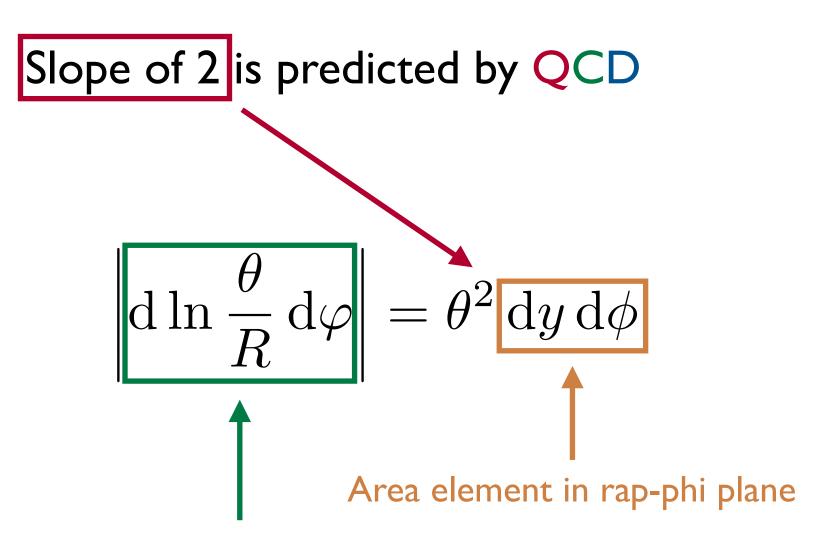




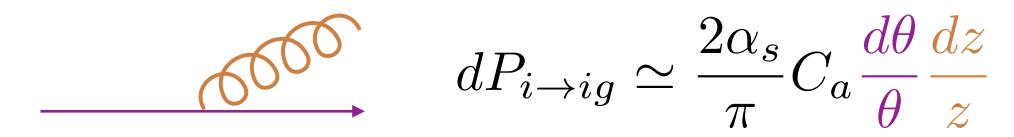


Quark vs. Gluon: Measuring EFN Filters

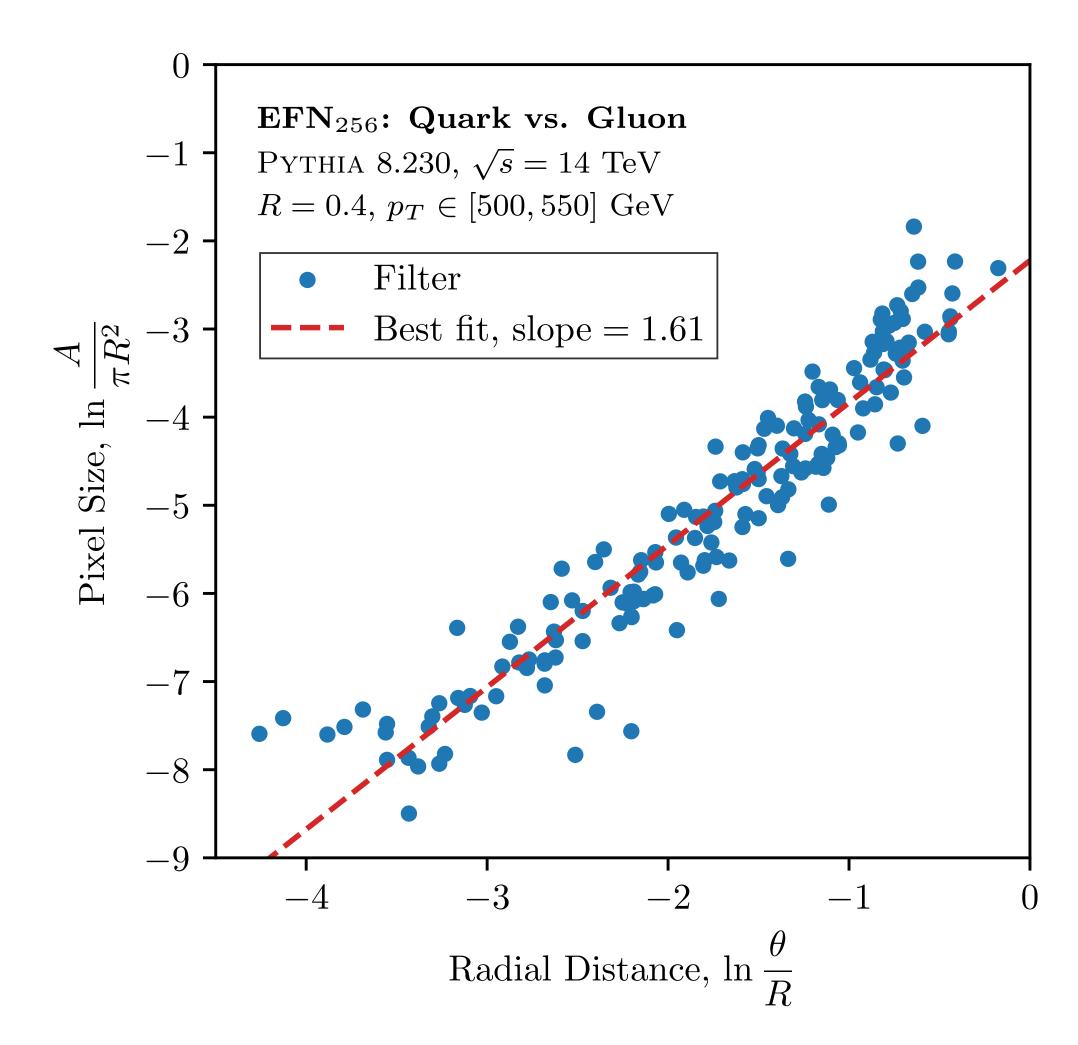
Energy Flow Network appears to have learned about the collinear singularity of QCD!



Emission plane area element

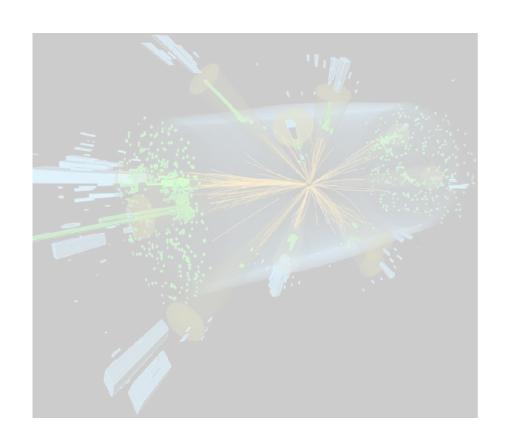


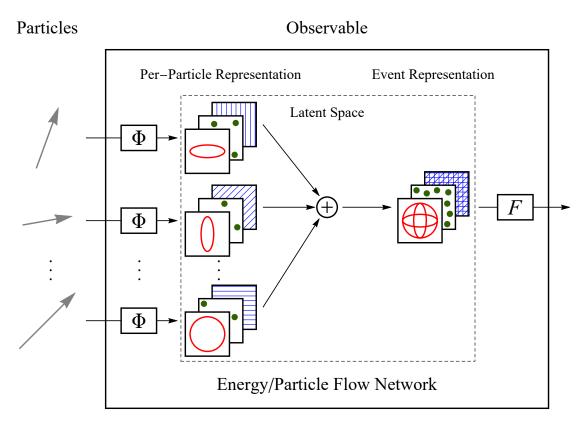
Altarelli-Parisi splitting function describes gluon emission



Power-law dependence between filter size and distance from center is observed

(Additional analysis of filters in backup)





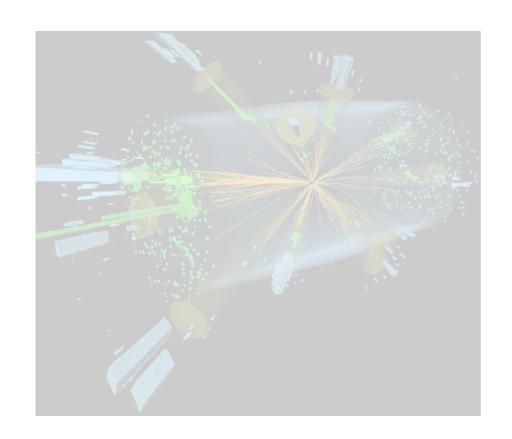


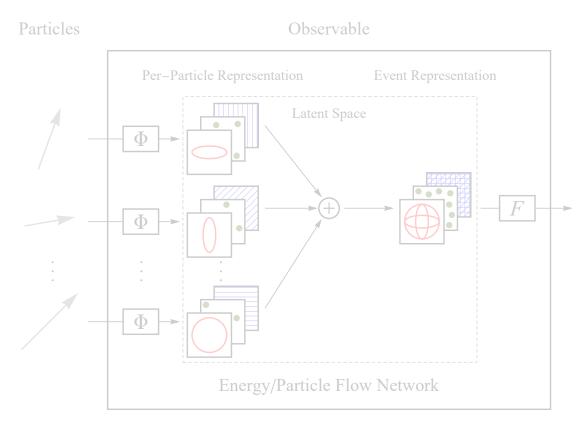
Particle Physics Fundamentals – Jets

Architectures for Colliders – EFNs/PFNs

Simple, extensible neural network architecture(s) for collider events

Statistical Deconvolution







Particle Physics Fundamentals – Jets

Jets are critical to the success of the modern collider program

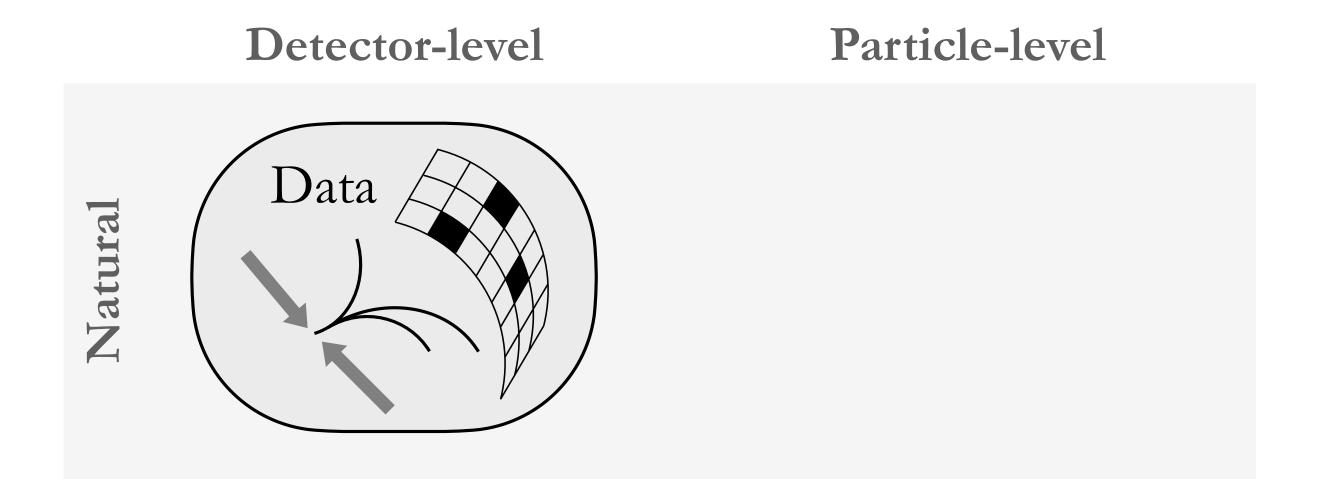
Architectures for Colliders – EFNs/PFNs

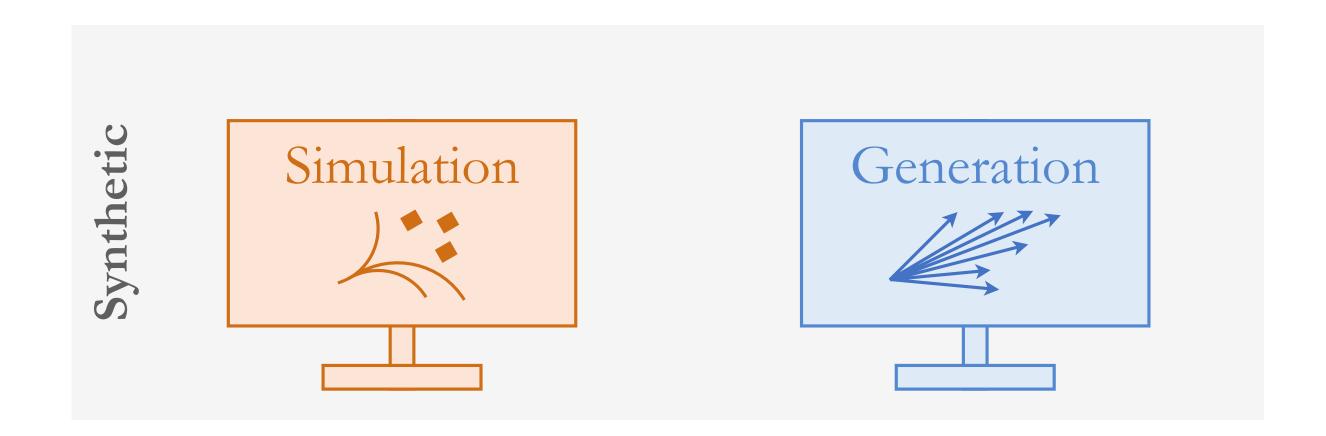
Simple, extensible neural network architecture(s) for collider events

Statistical Deconvolution

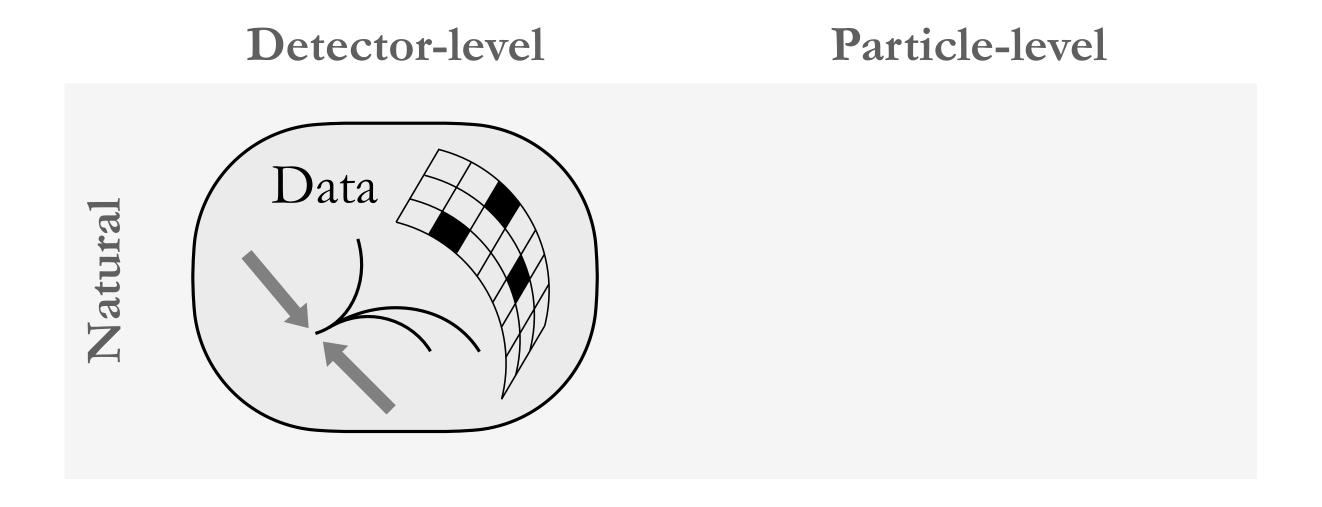
Can ML overcome the curse of dimensionality in correcting mis-measurements?

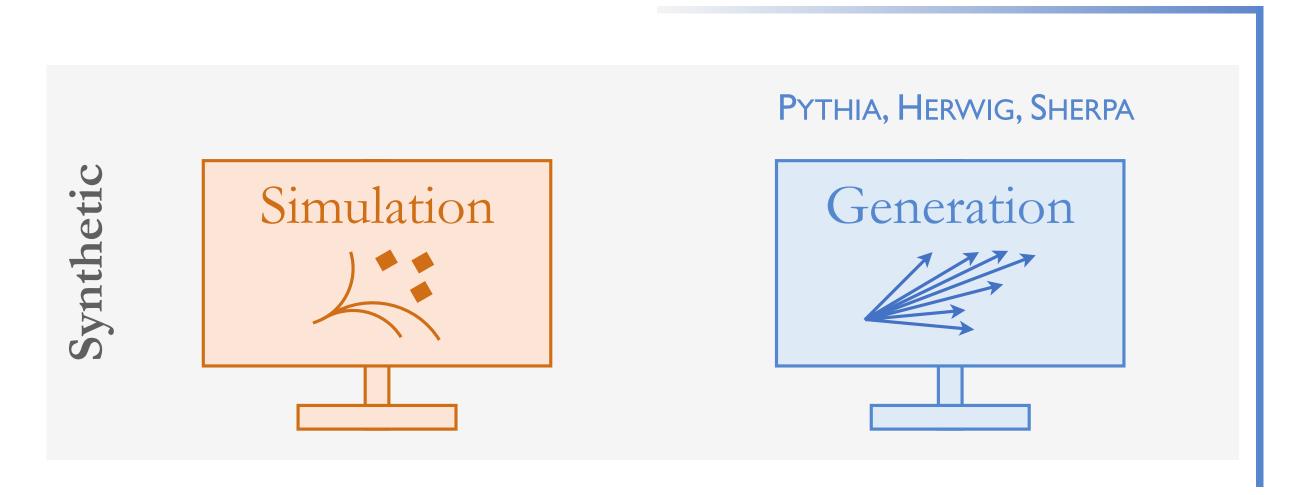
Measurements are affected by detector effects such as finite resolution, miscalibration, and limited acceptance



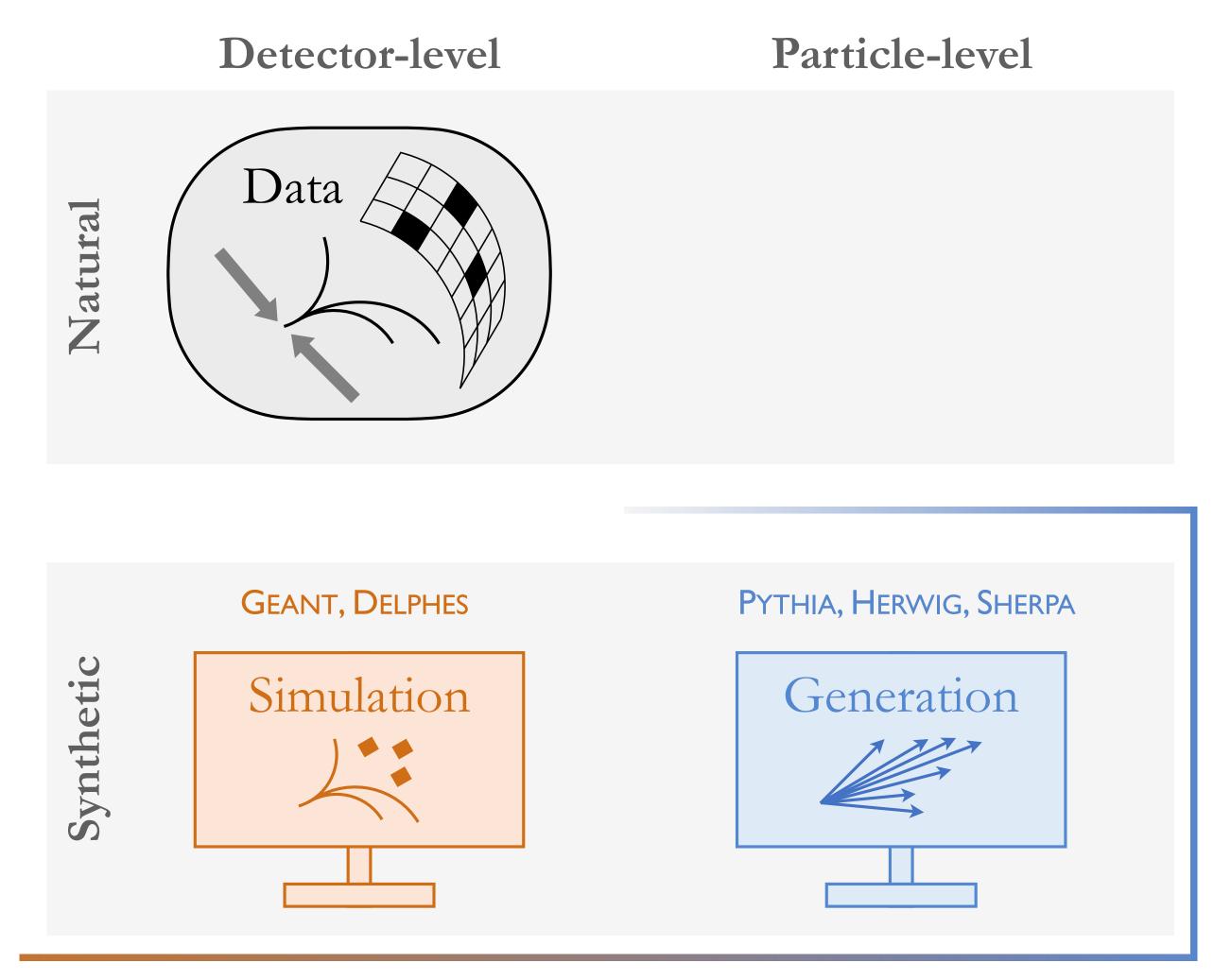


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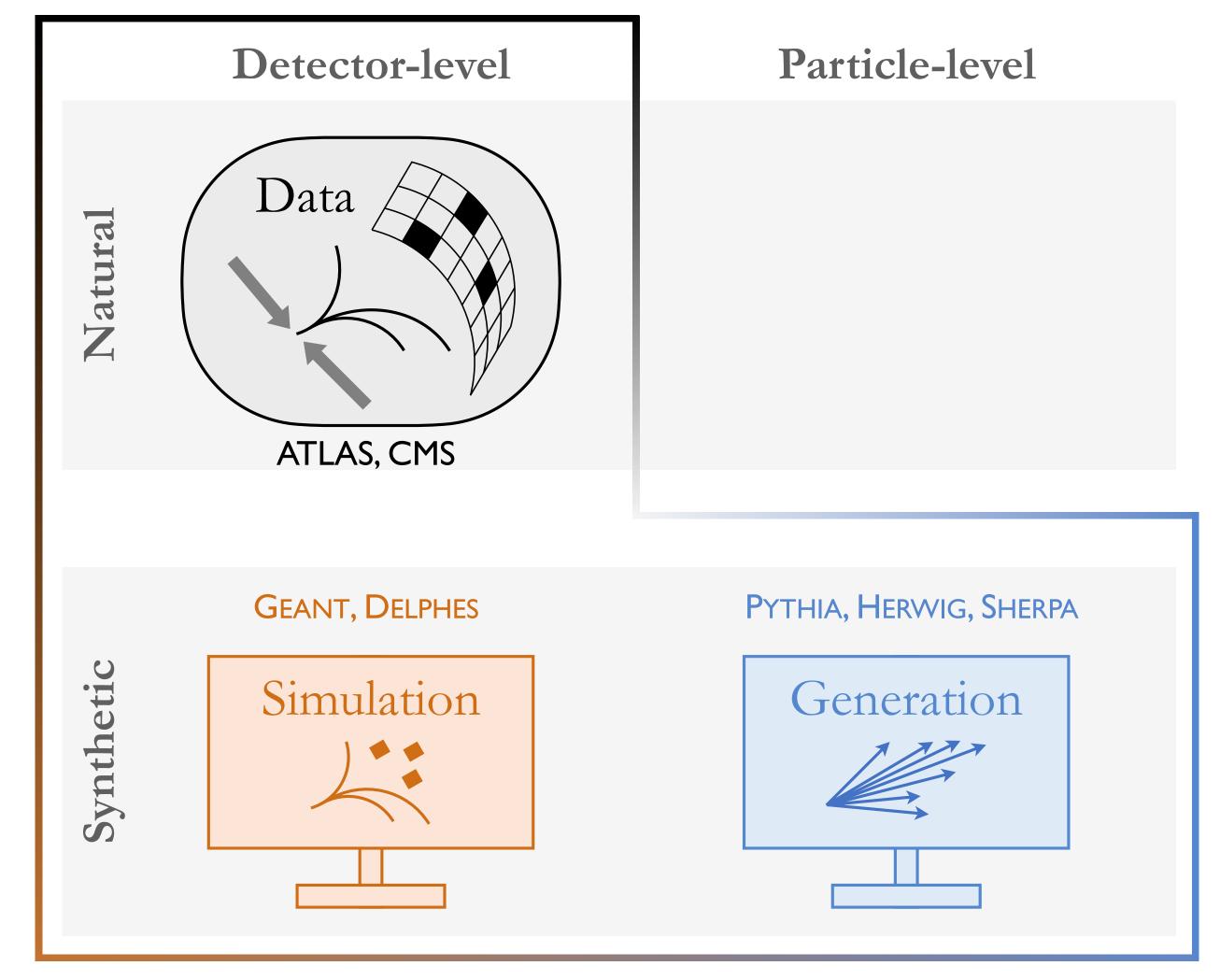


Measurements are affected by detector effects such as finite resolution, miscalibration, and limited acceptance



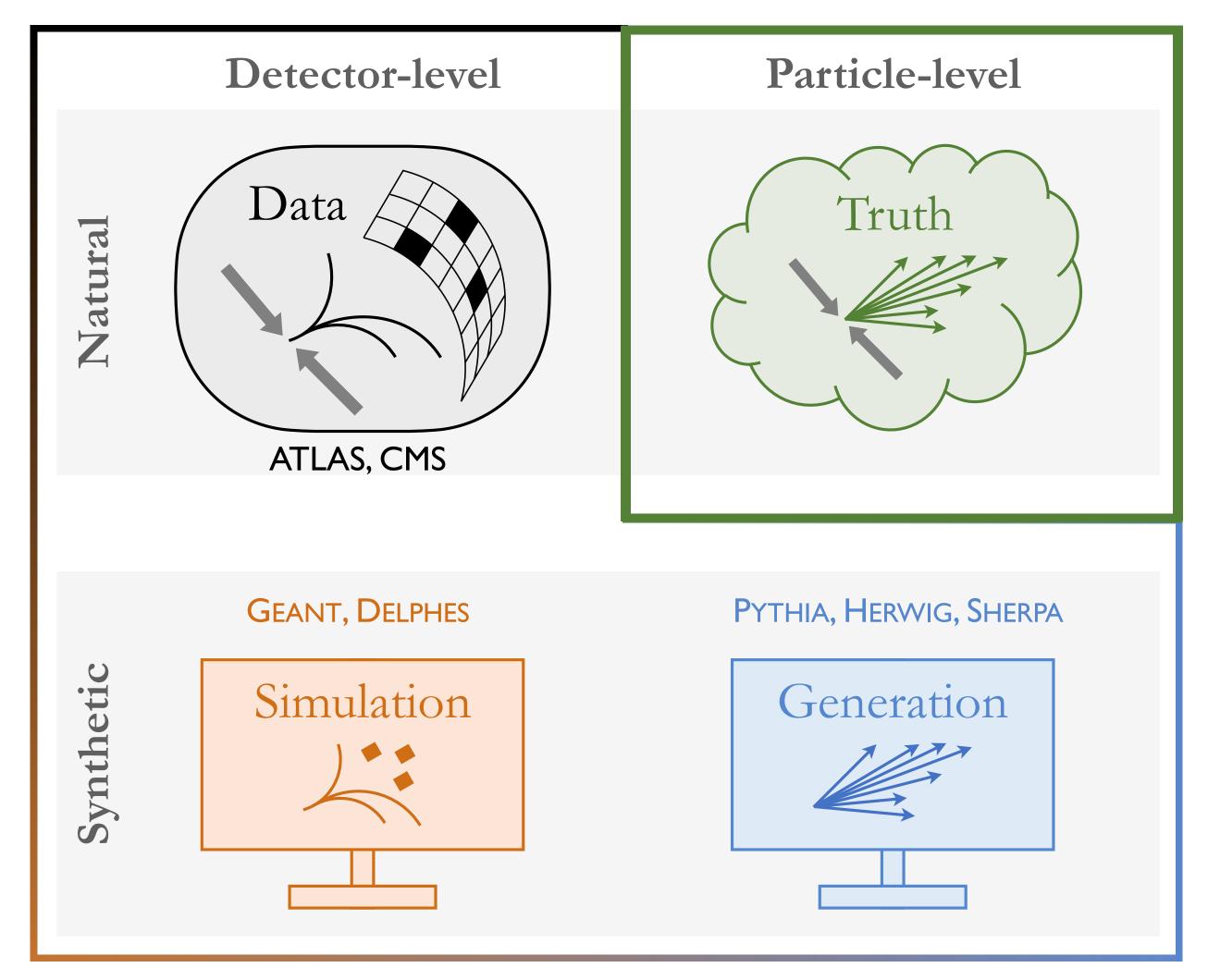
Learn detector response from trustable simulation

Measurements are affected by detector effects such as finite resolution, miscalibration, and limited acceptance



Learn detector response from trustable simulation

Measurements are affected by detector effects such as finite resolution, miscalibration, and limited acceptance

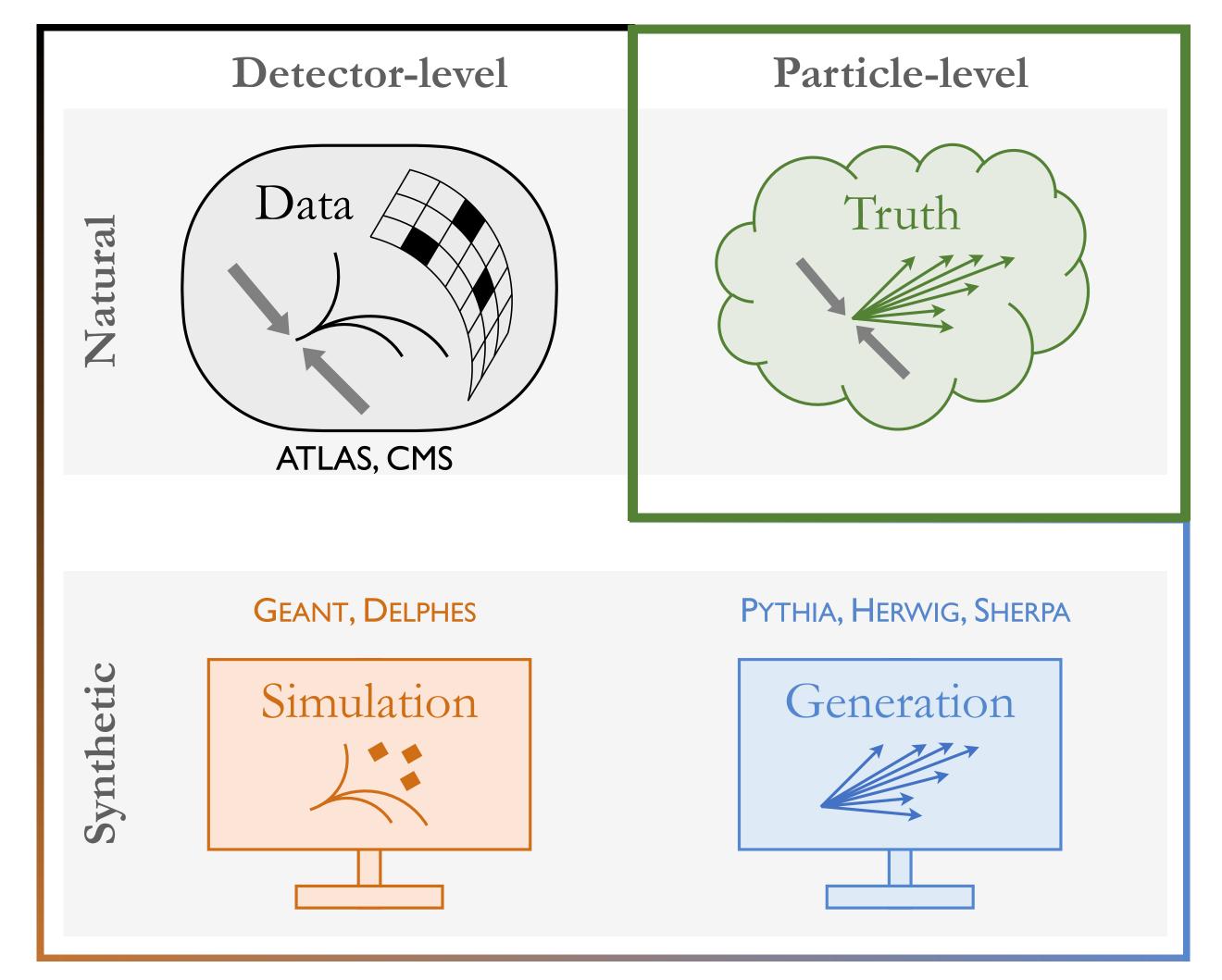


Truth-level measurements can be compared across experiments and to theoretical calculations

Goal of unfolding is to learn a particle-level model that reproduces the data

Learn detector response from trustable simulation

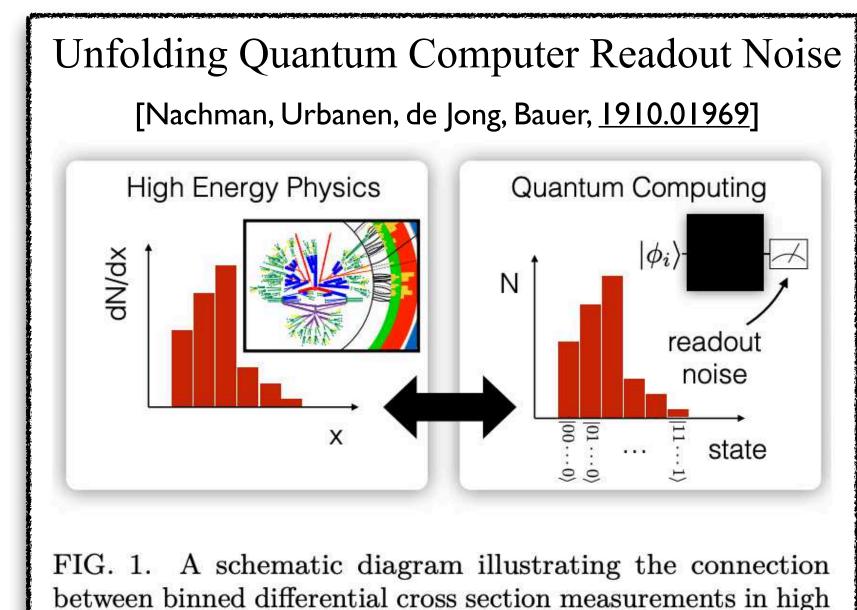
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Learn detector response from trustable simulation

Truth-level measurements can be compared across experiments and to theoretical calculations

Goal of unfolding is to learn a particle-level model that reproduces the data



Challenges with Traditional Unfolding

Previous methods explicitly rely on histograms

Binning fixed ahead of time, cannot be changed later Performance of method sensitive to binning

Limited number of observables

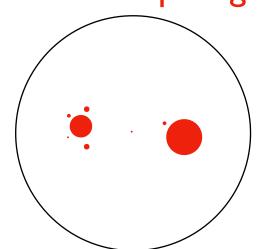
Binning induces curse of dimensionality

Response matrix depends on auxiliary features

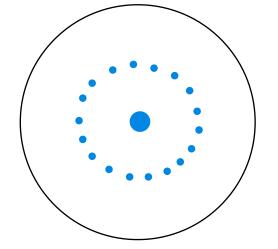
Detector-level quantity may not capture full detector effect

Example – Two jets acquiring the same mass in different ways

let 1



Two hard prongs Hard core, diffuse spray



Iterated Bayesian Unfolding (IBU)

also called Richardson-Lucy Deconvolution

Maximum likelihood, histogram-based unfolding method for a small number of observables

Choose observable(s) and binning at detector-level and particle-level

measured distribution: $m_i = \Pr(\text{measure } i)$ true distribution: $t_i^{(0)} = \Pr(\text{truth is } j)$

Calculate response matrix R_{ii} from generated/simulated pairs of events

$$R_{ij} = \Pr(\text{measure } i \mid \text{truth is } j)$$

Calculate new particle-level distribution using Bayes' theorem

$$t_{j}^{(n)} = \sum_{i} \Pr(\text{truth}_{n-1} \text{ is } j \mid \text{measure } i) \times \Pr(\text{measure } i)$$

$$= \sum_{i} \frac{R_{ij}t_{j}^{(n-1)}}{\sum_{k} R_{ik}t_{k}^{(n-1)}} \times m_{i}$$

Iterate procedure to remove dependence on prior

Likelihood Reweighting via Classification

Likelihood ratio is optimal binary classifier by Neyman-Pearson lemma

$$L[(w,X),(w',X')](x)=rac{p_{(w,X)}(x)}{p_{(w',X')}(x)}$$
 $X-\text{phase space}$ $X-\text{phase space}$

L – likelihood ratio

x – element of X

p – probability density

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Likelihood ratio is optimal binary classifier by Neyman-Pearson lemma

$$L[(w,X),(w',X')](x) = \frac{p_{(w,X)}(x)}{p_{(w',X')}(x)} \qquad \begin{array}{c} L - \text{likelihood rate} \\ w - \text{weights} \\ X - \text{phase space} \end{array}$$

L – likelihood ratio

x – element of X

p – probability density

Model output of a well-trained classifier accesses likelihood ratio

$$\mathsf{Model}[(w,X),(w',X')](x) \simeq \frac{L[(w,X),(w',X')](x)}{1+L[(w,X),(w',X')](x)} \qquad \text{Assuming softmax output, categorical cross-entropy loss}$$

[Cranmer, Pavez, Louppe, 1506.02169; Andreassen, Nachman, PRD 2020]

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[Cranmer, Pavez, Louppe, 1506.02169; Andreassen, Nachman, PRD 2020]

OmniFold repeatedly reweights one weighted sample (A) to another (B)

Likelihood reweighting requires effective classification of events

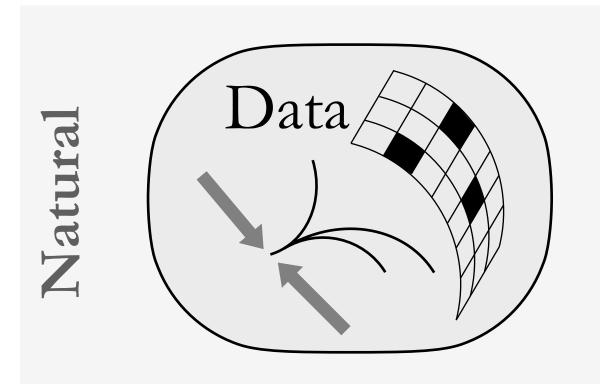


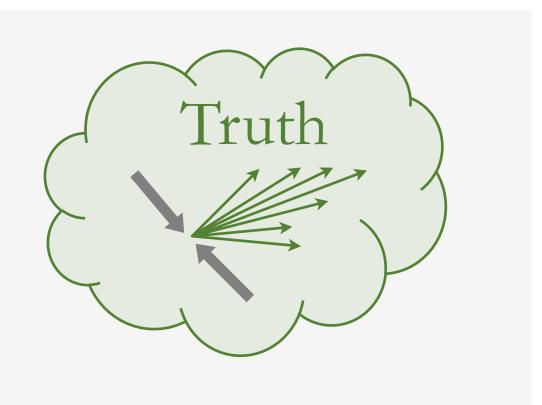
OmniFold weights particle-level Gen to be consistent with Data once passed through the detector

[Andreassen, PTK, Metodiev, Nachman, Thaler, PRL 2020]

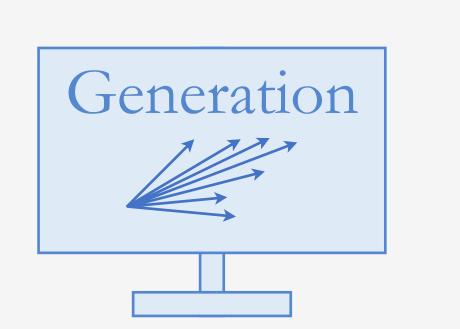
Detector-level







Simulation





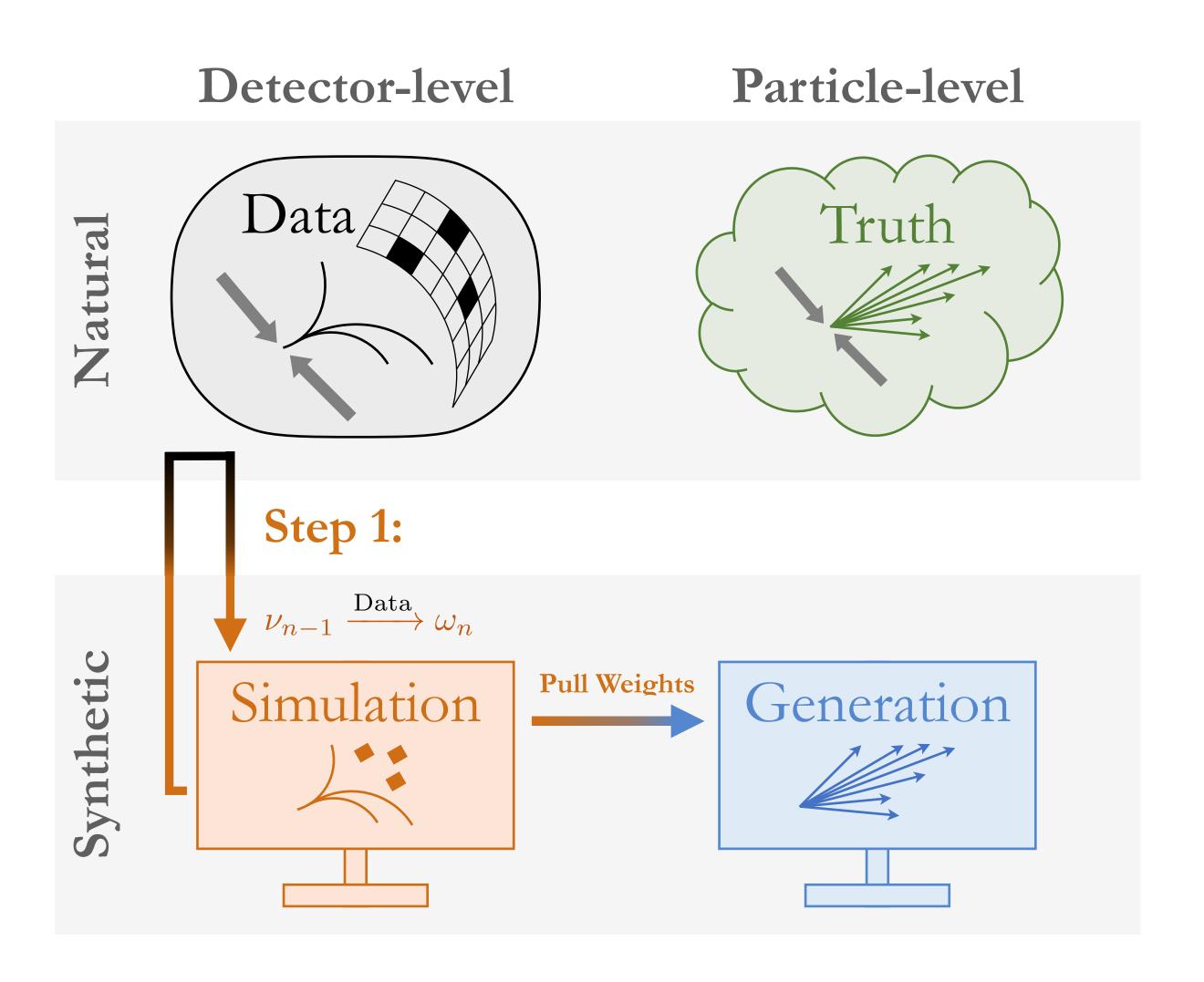
OmniFold weights particle-level Gen to be consistent with Data once passed through the detector

Step 1

Reweights Sim_{n-1} to data, pulls weights back to particle-level Gen_{n-1}

Incorporates the response matrix

[Andreassen, PTK, Metodiev, Nachman, Thaler, PRL 2020]





OmniFold weights particle-level Gen to be consistent with Data once passed through the detector

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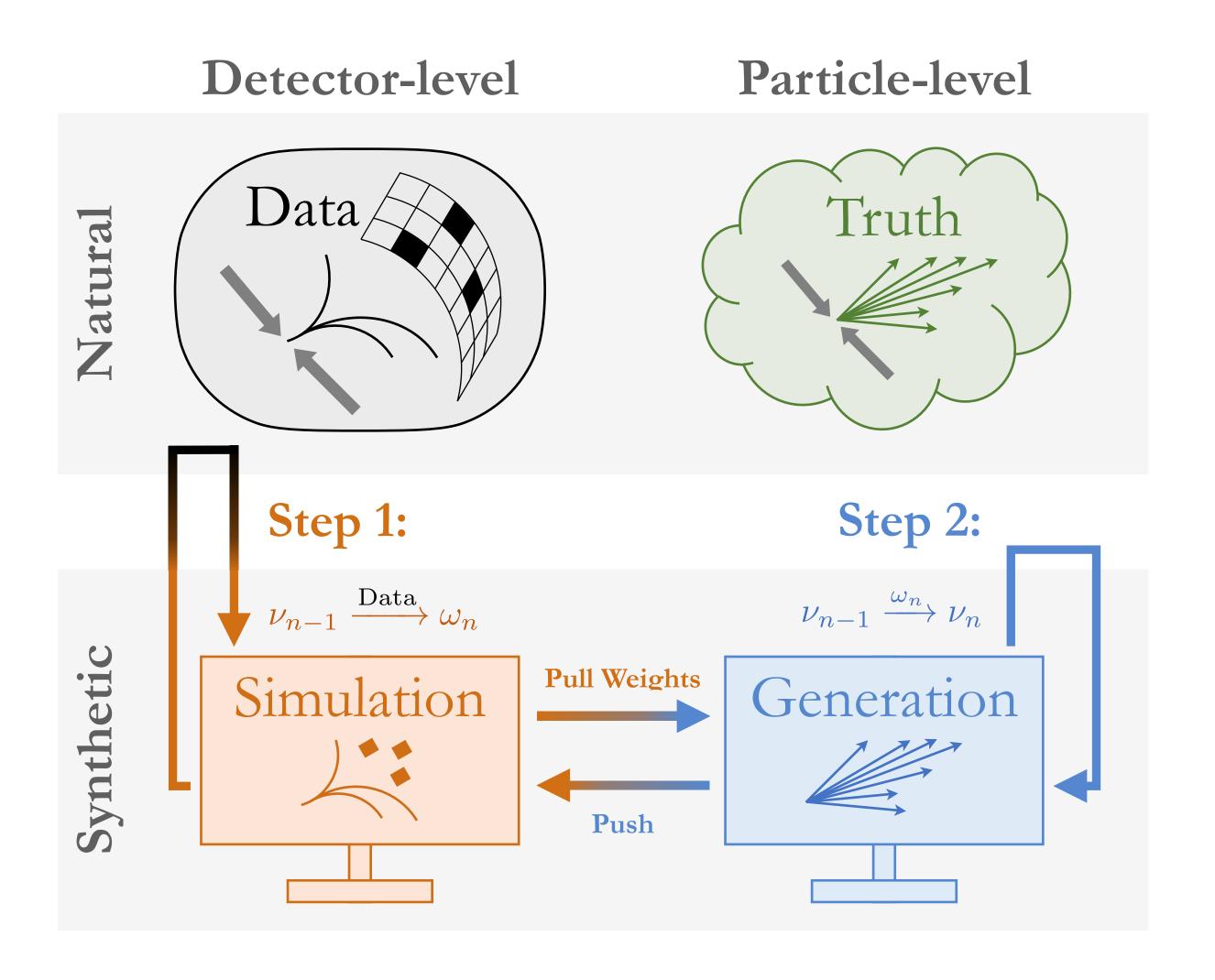
Incorporates the response matrix

Step 2

Reweights Gen_{n-1} to (step 1)-weighted gen_{n-1}, pushes weights to detector-level Sim_n

Constructs valid particle-level function by averaging gen-level weights

[Andreassen, PTK, Metodiev, Nachman, Thaler, PRL 2020]





[Andreassen, PTK, Metodiev, Nachman, Thaler, PRL 2020]

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OmniFold

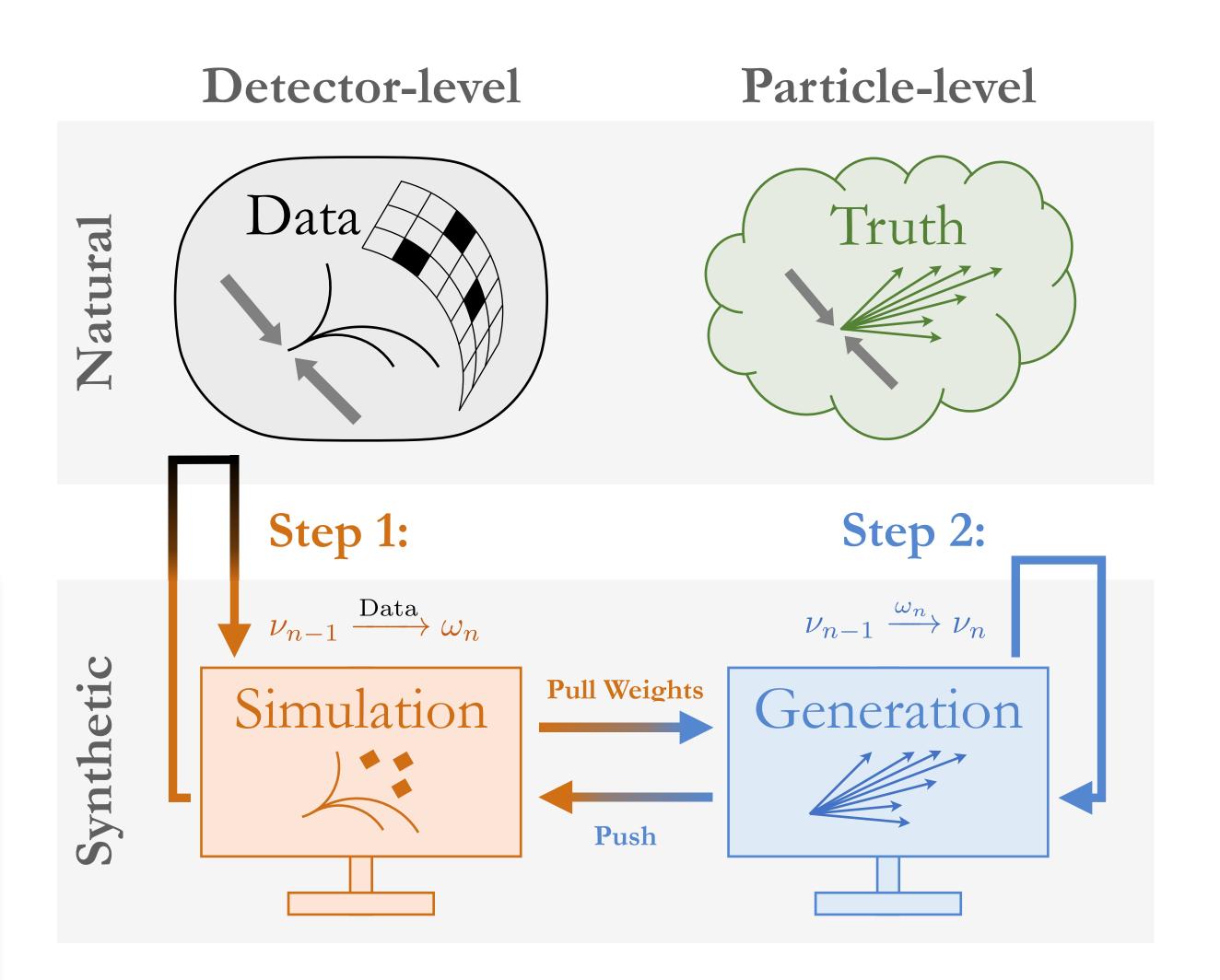
Step 1 –
$$\omega_n(m) = \nu_{n-1}^{\text{push}} \times L[(1, \text{Data}), (\nu_{n-1}^{\text{push}}, \text{Sim})](m)$$

Step 2 -
$$\nu_n(t) = \nu_{n-1}(t) \times L[(\omega_n^{\text{pull}}, \text{Gen}), (\nu_{n-1}, \text{Gen})](t)$$

Unfold any* observable $p_{Gen}(t)$ using universal weights $\nu_n(t)$

$$p_{\text{unfolded}}^{(n)}(t) = \nu_n(t) \times p_{\text{Gen}}(t)$$

*Observables should be chosen responsibly



Simultaneously Unfolding All Observables - OmniFold

OmniFold weights particle-level Gen to be consistent

[Andreassen, PTK, Metodiev, Nachman, Thaler, PRL 2020]

Rev

The Mountain sat upon the Plain In his tremendous Chair — His observation OmniFold, His inquest, everywhere —

The Seasons played around his knees Like Children round a sire – Grandfather of the Days is He Of Dawn, the Ancestor –

Emily Dickinson, #975





Testing OmniFold -Z +Jet Case Study

[Andreassen, PTK, Metodiev, Nachman, Thaler, PRL 2020]



MC – PYTHIA 8.243, tune 26

1.6 million events each after cuts

Detector Simulation
CMS-like detector – DELPHES 3.4.2

Jets

Anti- k_T , R = 0.4 — FASTJET 3.3.2 $p_T^Z > 200$ GeV, assume excellent muon detector resolution

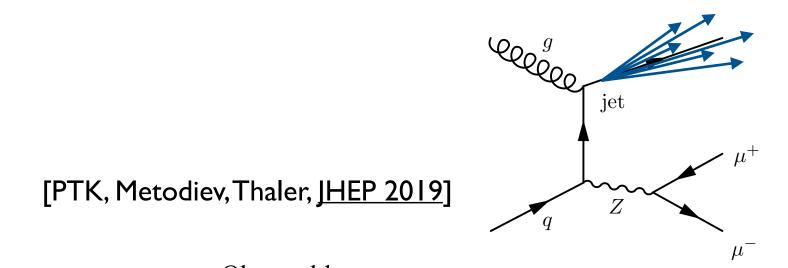
Datasets publicly available

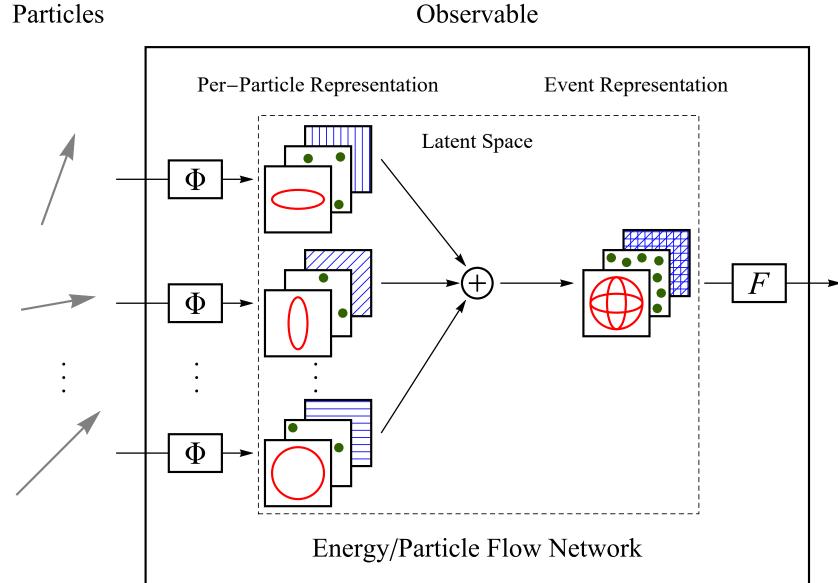
- -With two additional Pythia tunes
- -Accessible via **EnergyFlow**



OmniFold Binder Demo

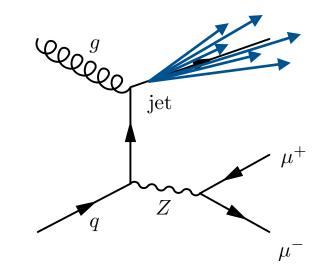






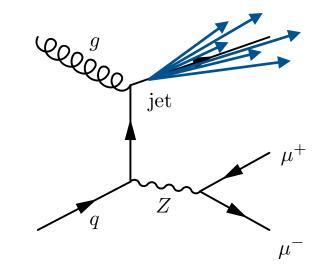
Particle Flow Network (PFN) architecture processes full radiation pattern of the event

- PFN-Ex: (p_T, y, ϕ, PID) input features
- $-\Phi: (100, 100, 256)$ dense layers
- *F* : (100,100,100) dense layers
- ReLU activations, softmax output
- Categorical cross-entropy loss
- 20% validation sample
- 10 epoch patience



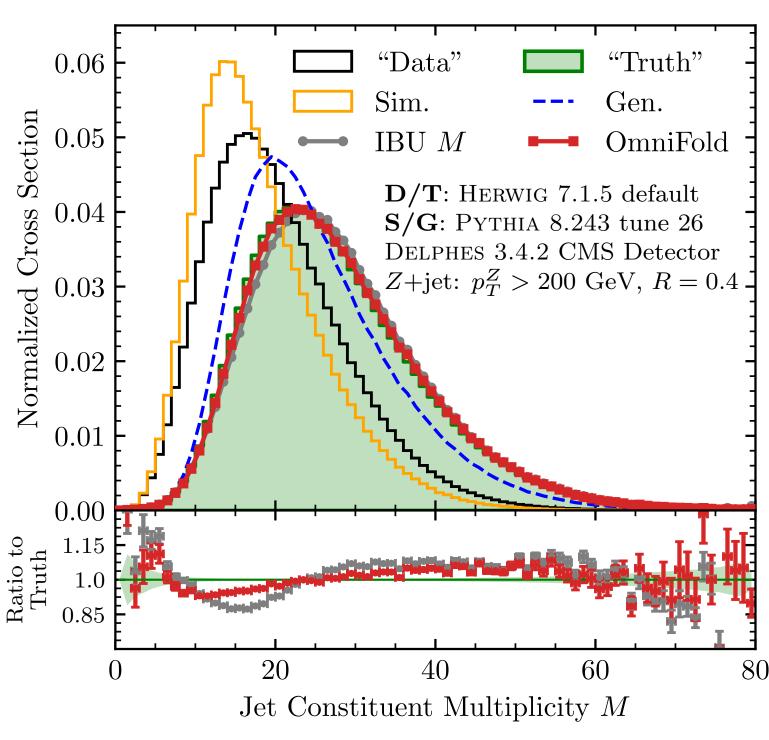
Single OmniFold instantiation vs. separate instantiations of IBU

Successful unfolding means IBU/OmniFold should approach Truth



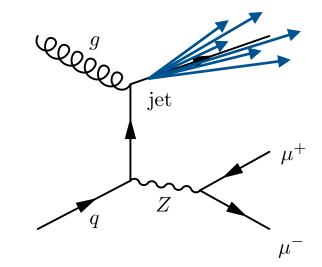
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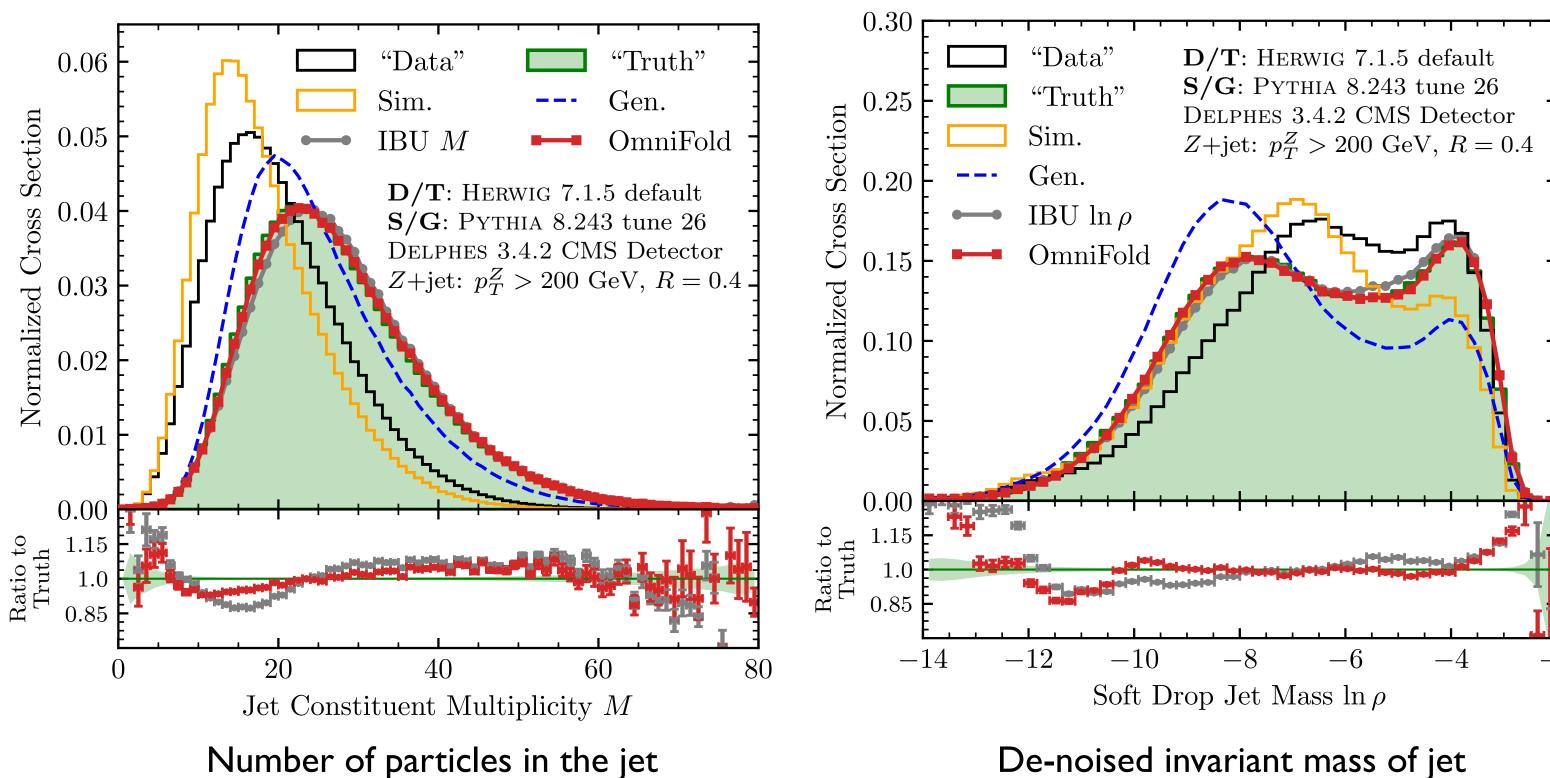
Number of particles in the jet

OmniFold equals or outperforms IBU



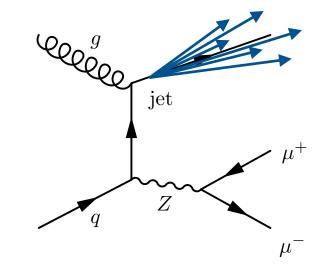
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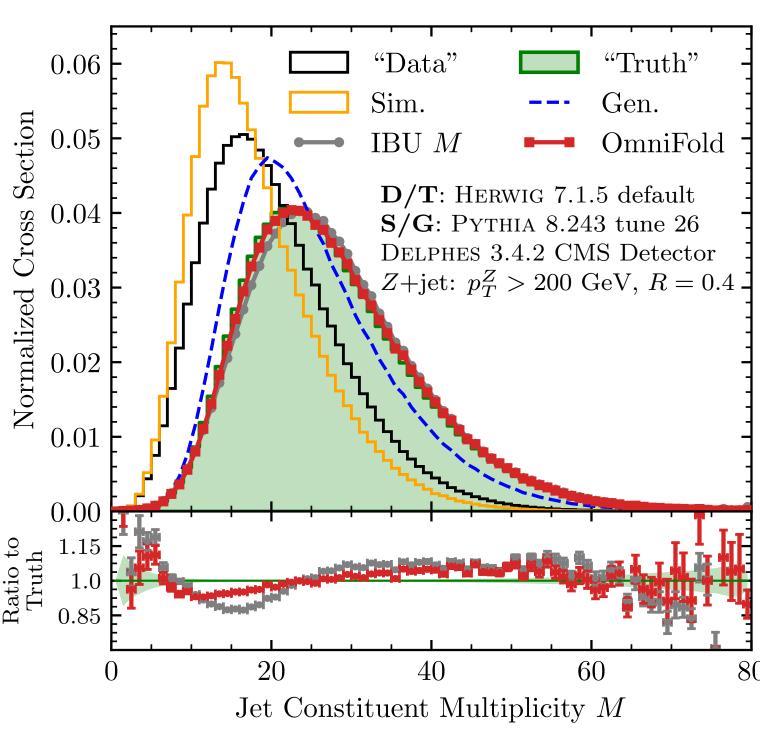
De-noised invariant mass of jet

OmniFold equals or outperforms IBU

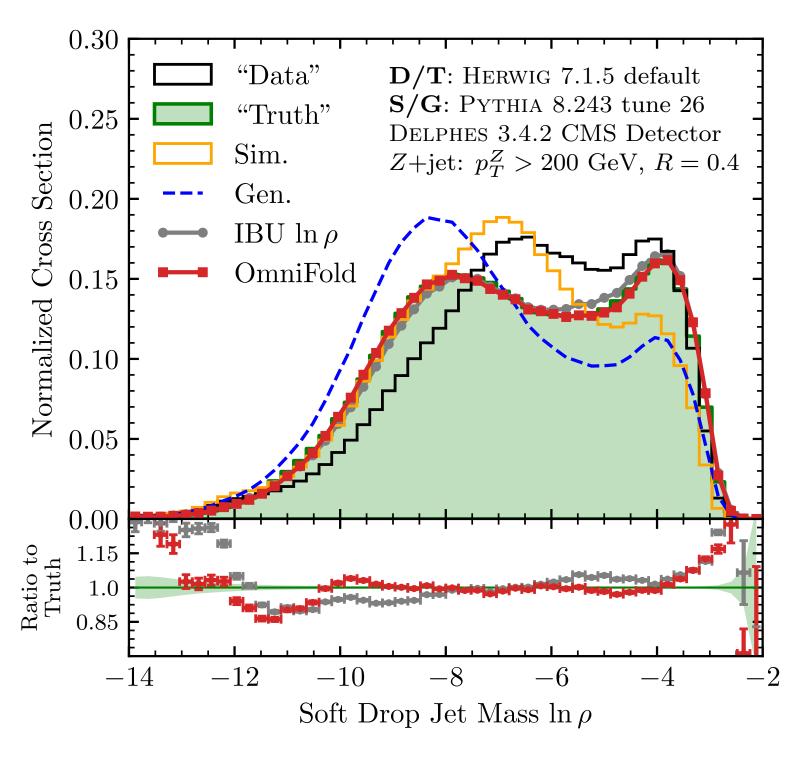


Single OmniFold instantiation vs. separate instantiations of IBU

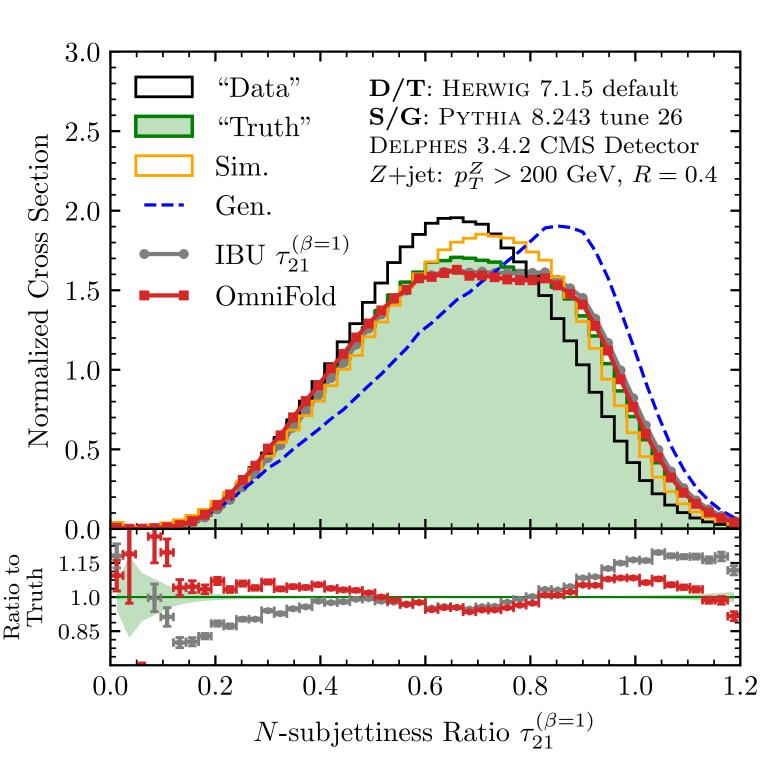
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Number of particles in the jet



De-noised invariant mass of jet



Ratio of "two-pronginess" to "one-pronginess"

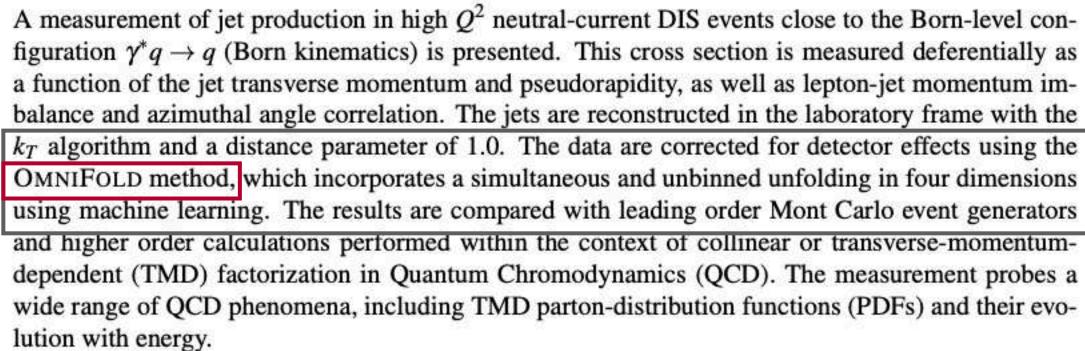
OmniFold equals or outperforms IBU

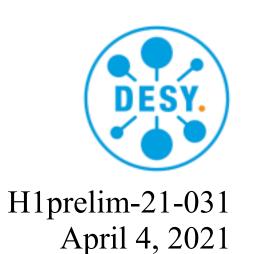
0.06 0.010.00 Jet Con

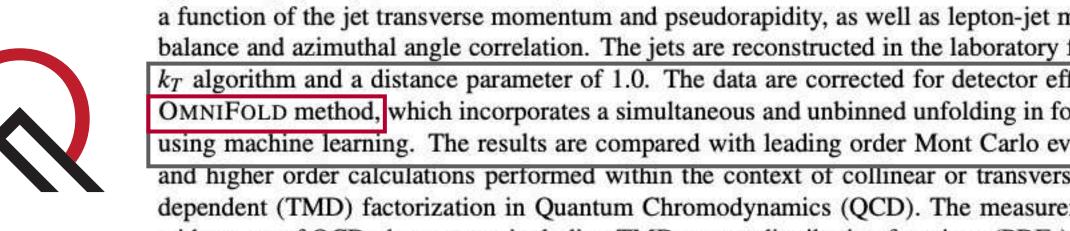
Measurement of lepton-jet correlations in high Q^2 neutral-current DIS with the H1 detector at HERA

The H1 Collaboration

Abstract







First application of OmniFold by an experimental collaboration!

In progress — OmniFolding jets in CMS Open Data to extract quark/gluon jet distributions [PTK, Kryhin, Thaler, to appear soon]

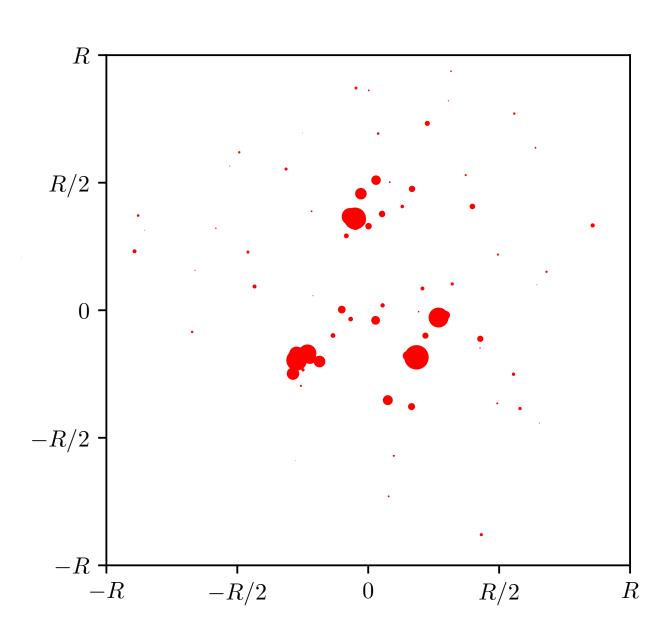
pronginess" onginess"

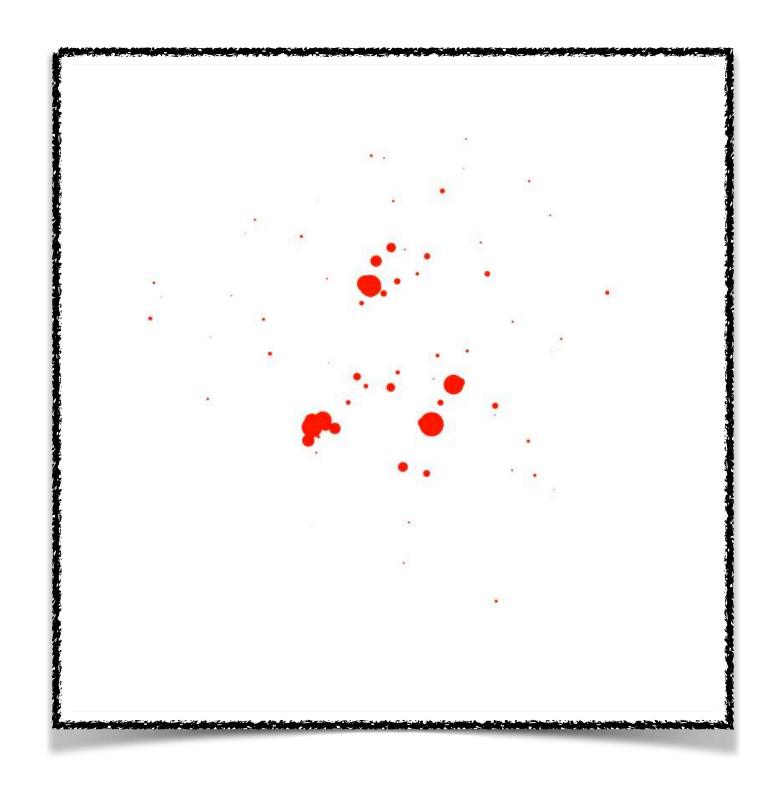
Ratio $au_{21}^{(\beta=1)}$

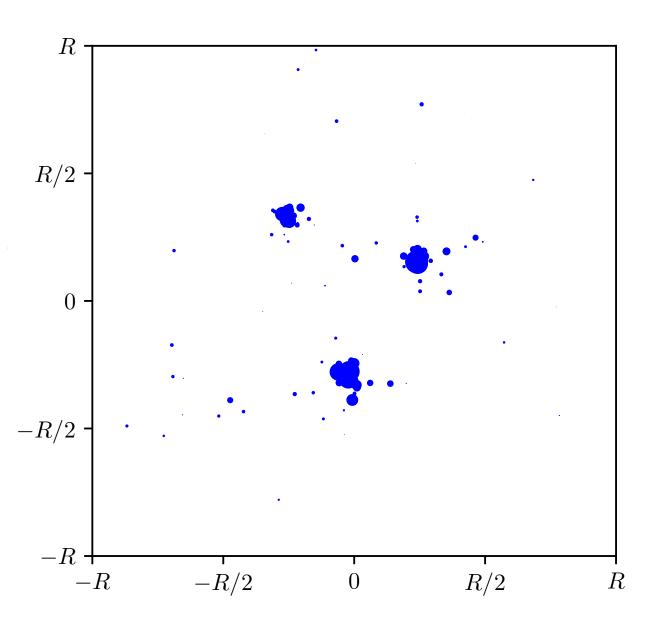
Number

Optimal Transport in Particle Physics

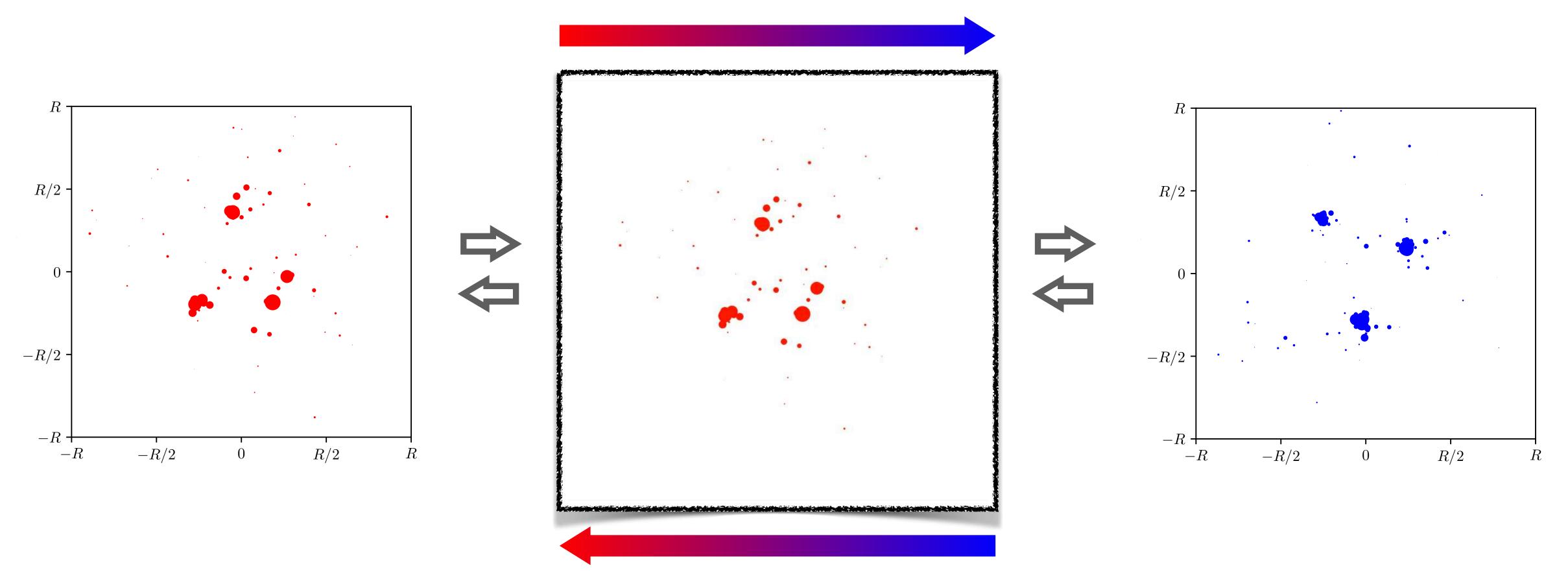
Optimal transport minimizes the "work" (stuff x distance) required to transport supply to demand

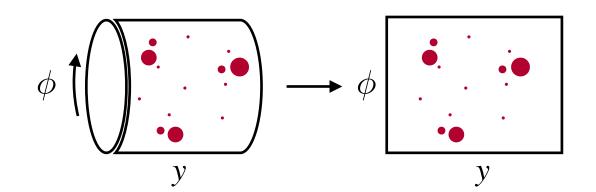




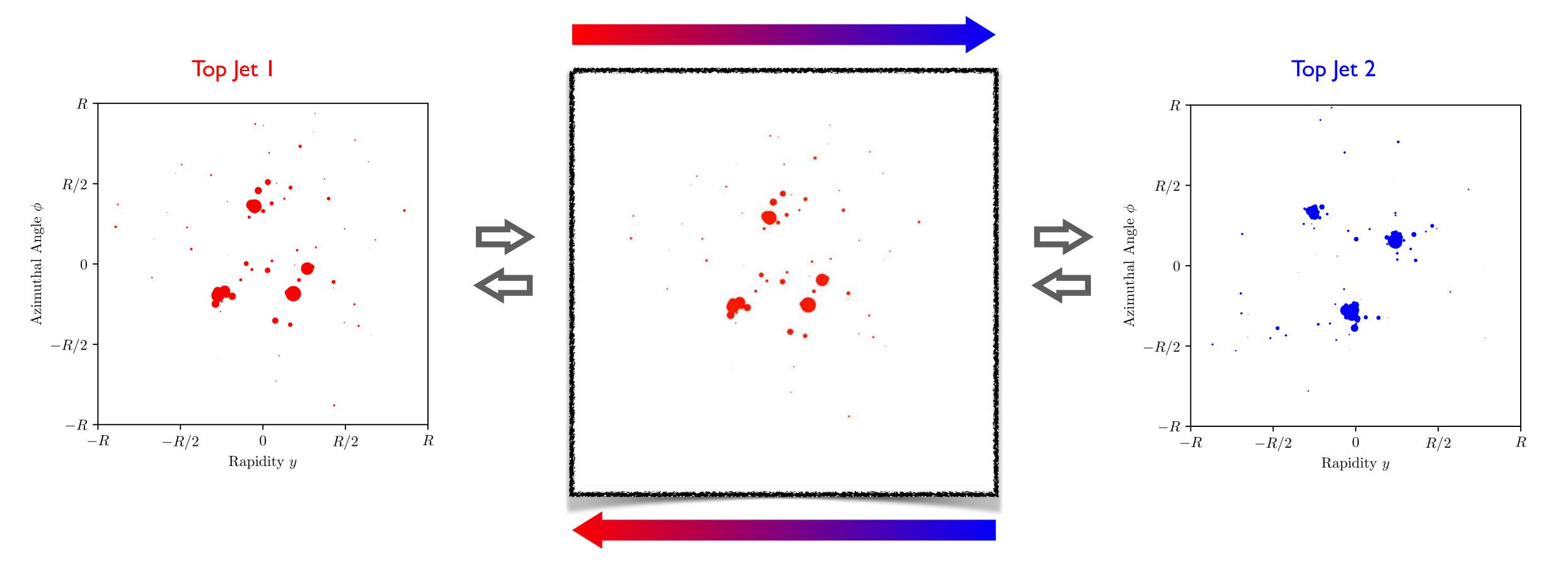


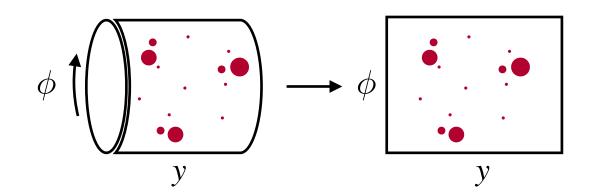
Optimal transport minimizes the "work" (stuff x distance) required to transport supply to demand



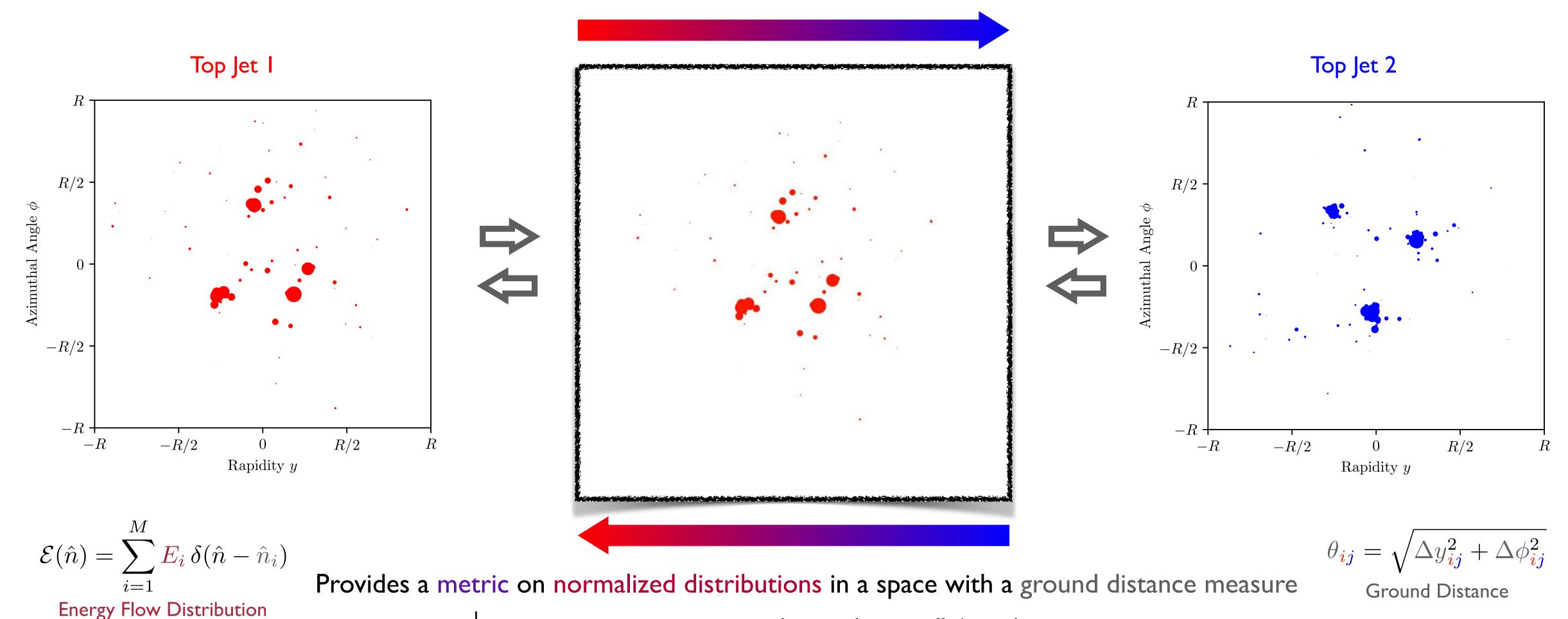


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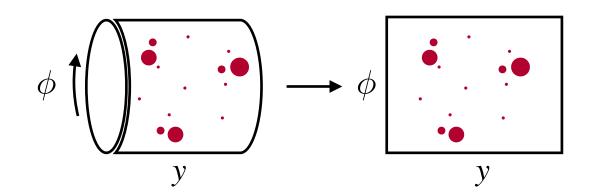




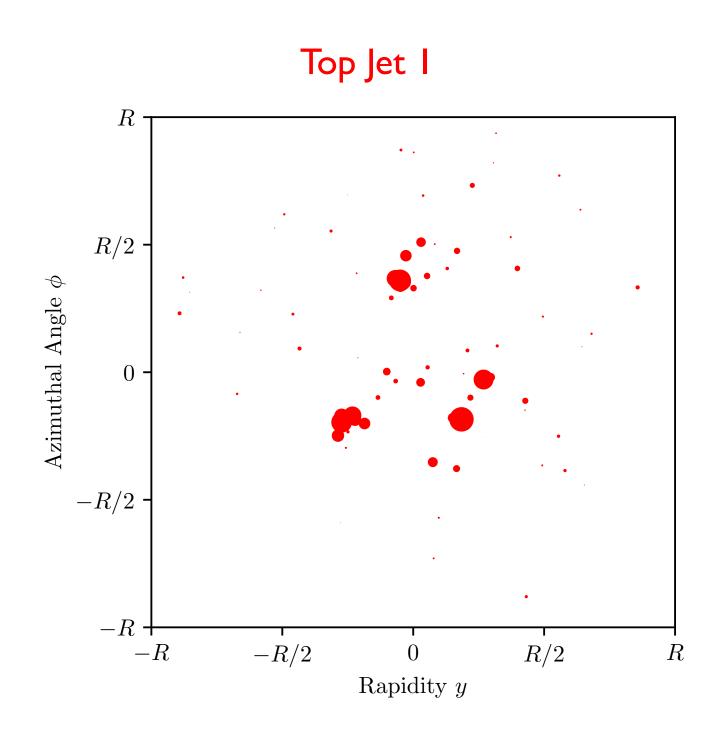
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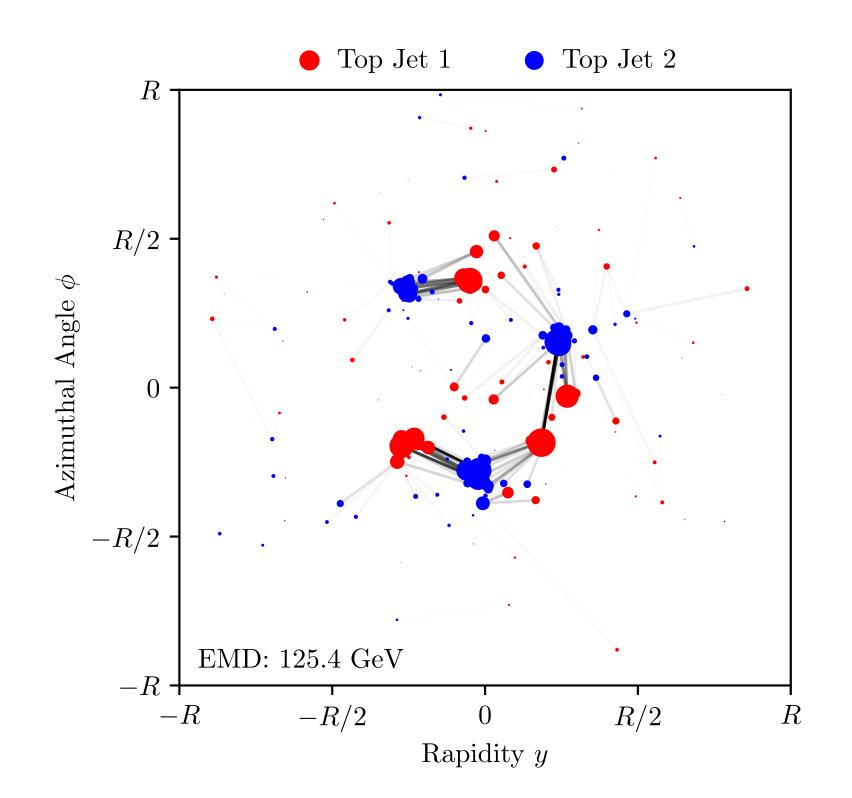


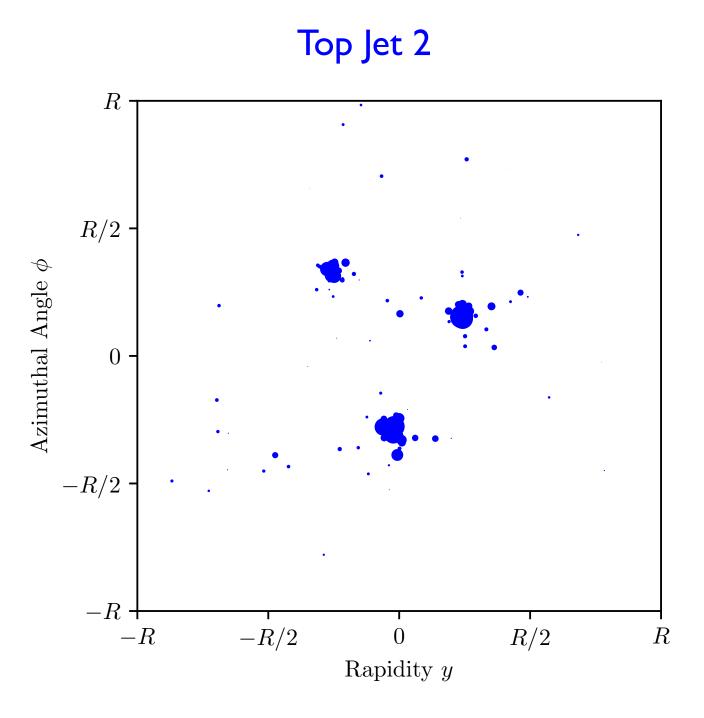
symmetric, non-negative, triangle inequality, zero iff identical



Optimal transport minimizes the "work" (stuff x distance) required to transport supply to demand







$$\mathcal{E}(\hat{n}) = \sum_{i=1}^{M} \mathbf{E}_{i} \, \delta(\hat{n} - \hat{n}_{i})$$

Energy Flow Distribution

Provides a metric on normalized distributions in a space with a ground distance measure

 $\theta_{\pmb{i}\pmb{j}} = \sqrt{\Delta y_{\pmb{i}\pmb{j}}^2 + \Delta \phi_{\pmb{i}\pmb{j}}^2}$ Ground Distance

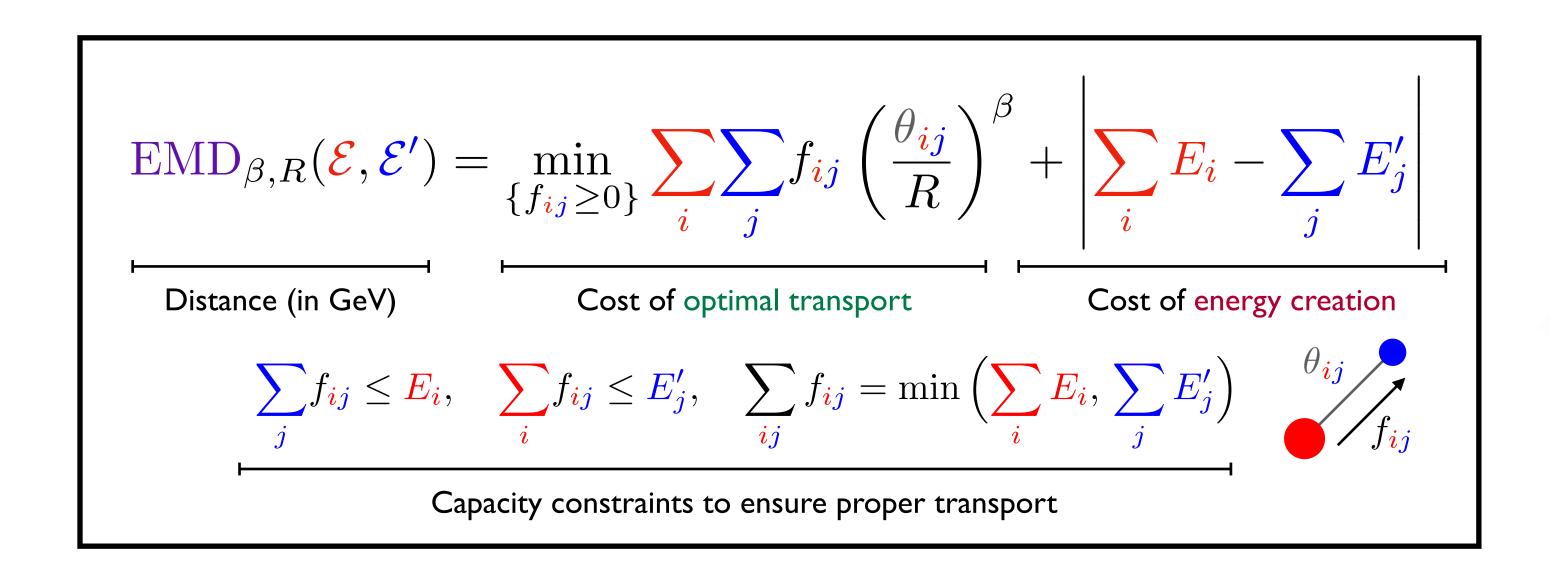
symmetric, non-negative, triangle inequality, zero iff identical

The Energy Mover's Distance (EMD)

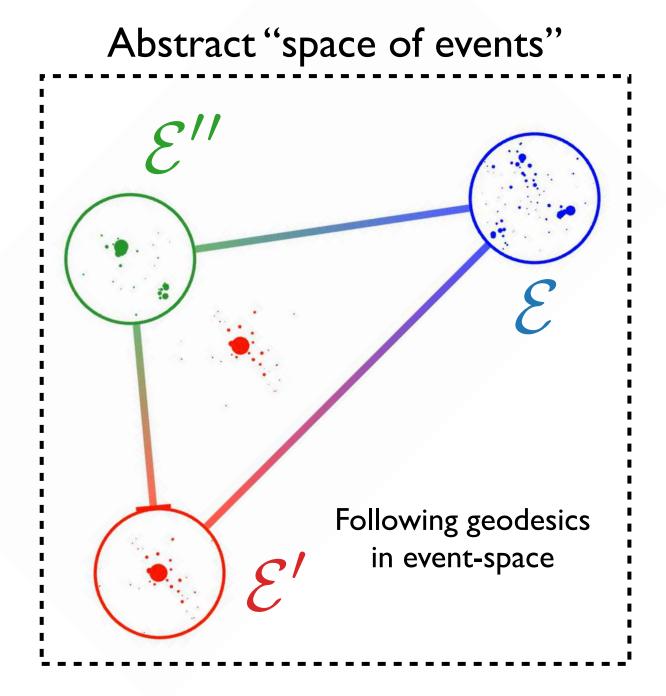
[PTK, Metodiev, Thaler, PRL 2019 (editors' suggestion), Featured in Physics Magazine; PTK, Metodiev, Thaler, JHEP 2020;

EnergyFlow and **Wasserstein** Python Packages]

EMD between energy flows defines a metric on the space of events



R: controls cost of transporting energy vs. destroying/creating it β : angular weighting exponent



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

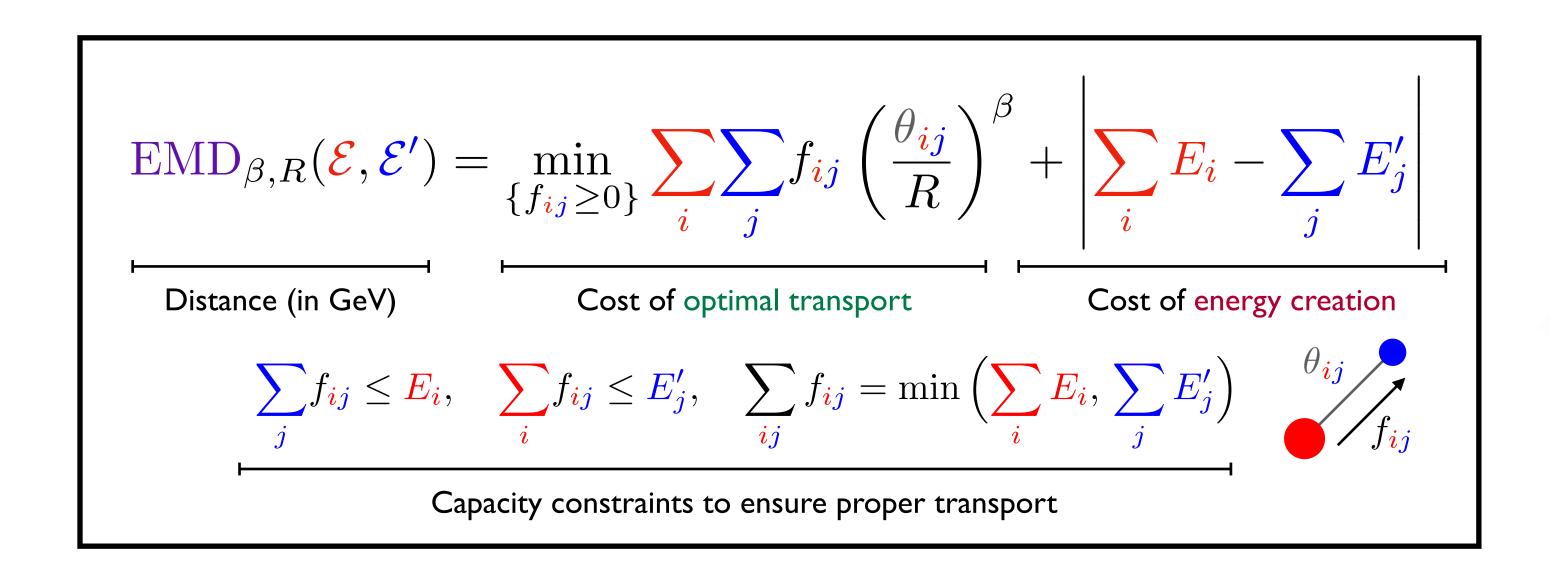
Triangle inequality satisfied for $R \ge d_{\max}/2$ i.e. $R \ge$ jet radius for conical jets

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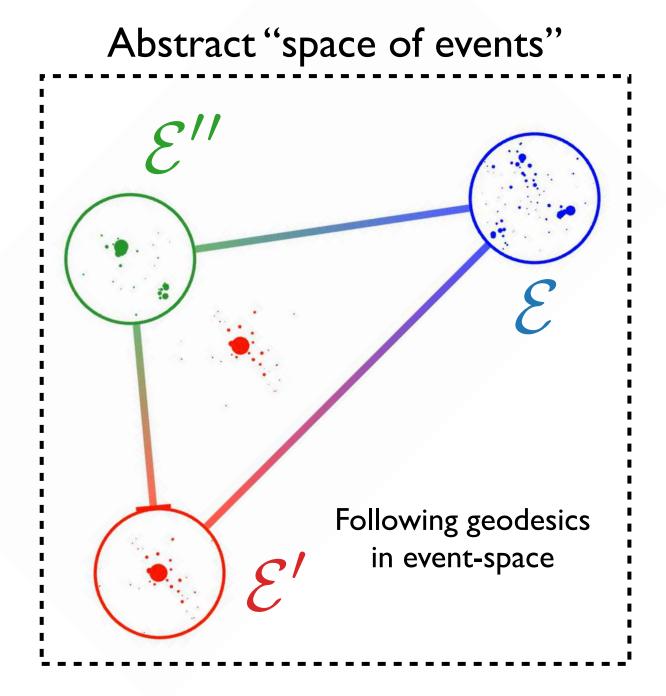
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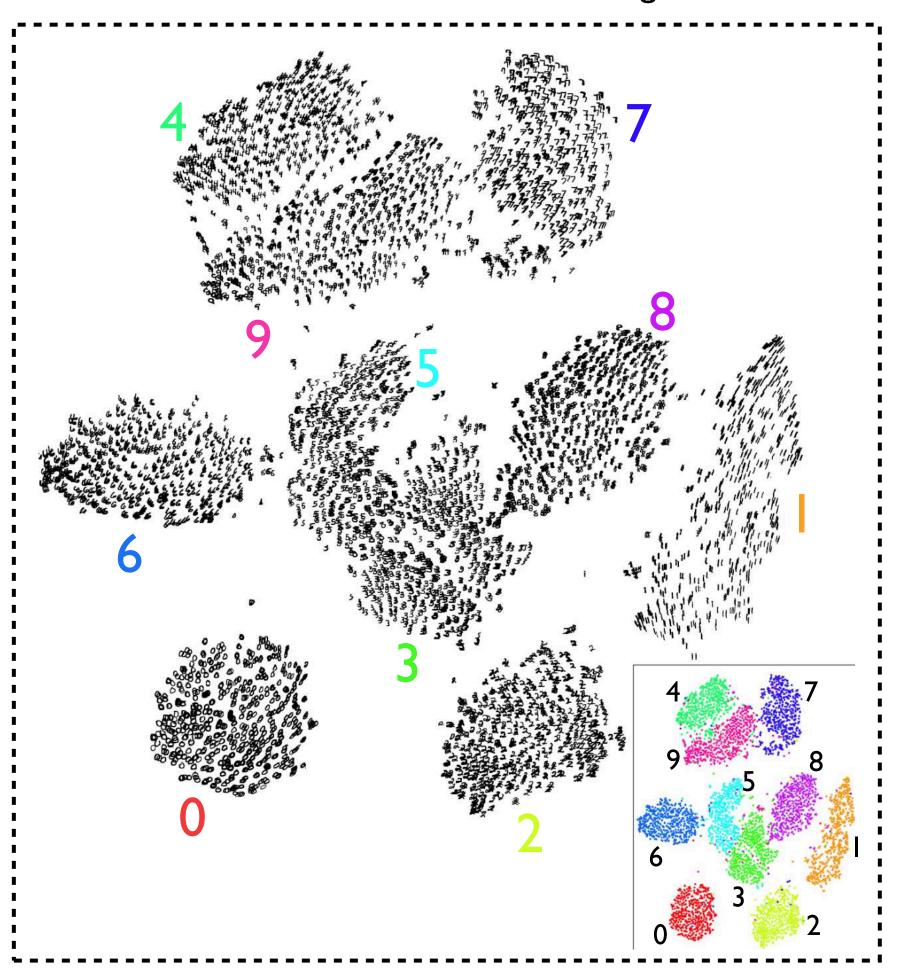
Triangle inequality satisfied for $R \ge d_{\max}/2$ i.e. $R \ge$ jet radius for conical jets

Visualizing Geometry in the Space of Events

[PTK, Mastandrea, Metodiev, Naik, Thaler, PRD 2019; code and datasets at energyflow.network]

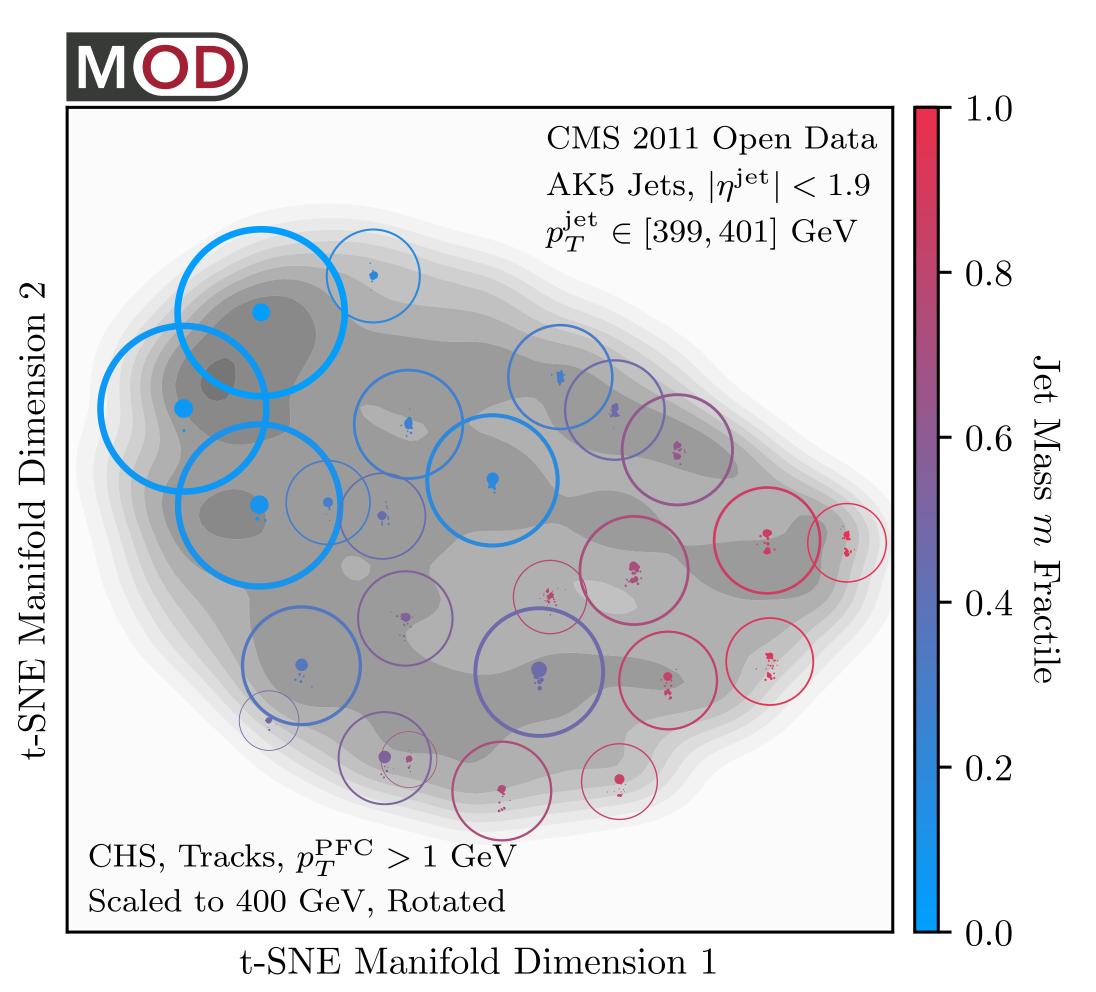
t-Distributed Stochastic Neighbor Embedding (t-SNE)

MNIST handwritten digits



[L. van der Maaten, G. Hinton, JMLR 2008]

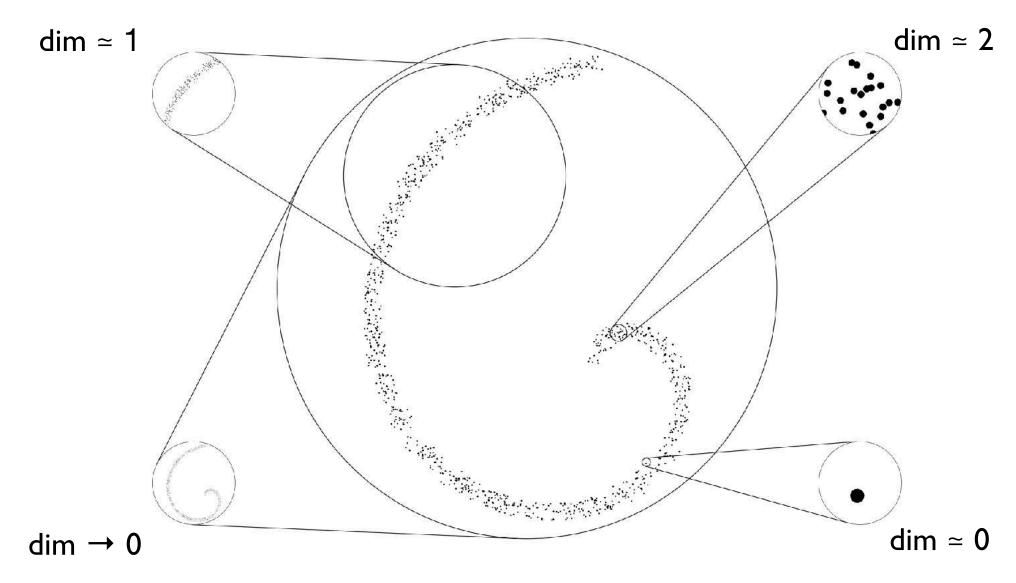
Jets from the CMS 2011 Open Data



25 most representative jets ("medoids")
Size is proportional to cross section associated to that medoid

Unfolding Beyond Observables

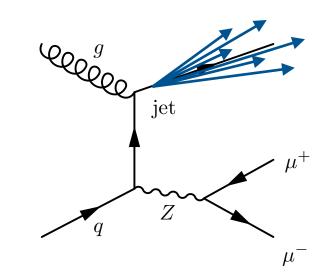
Correlation dimension: how does the # of elements within a ball of size Q change?

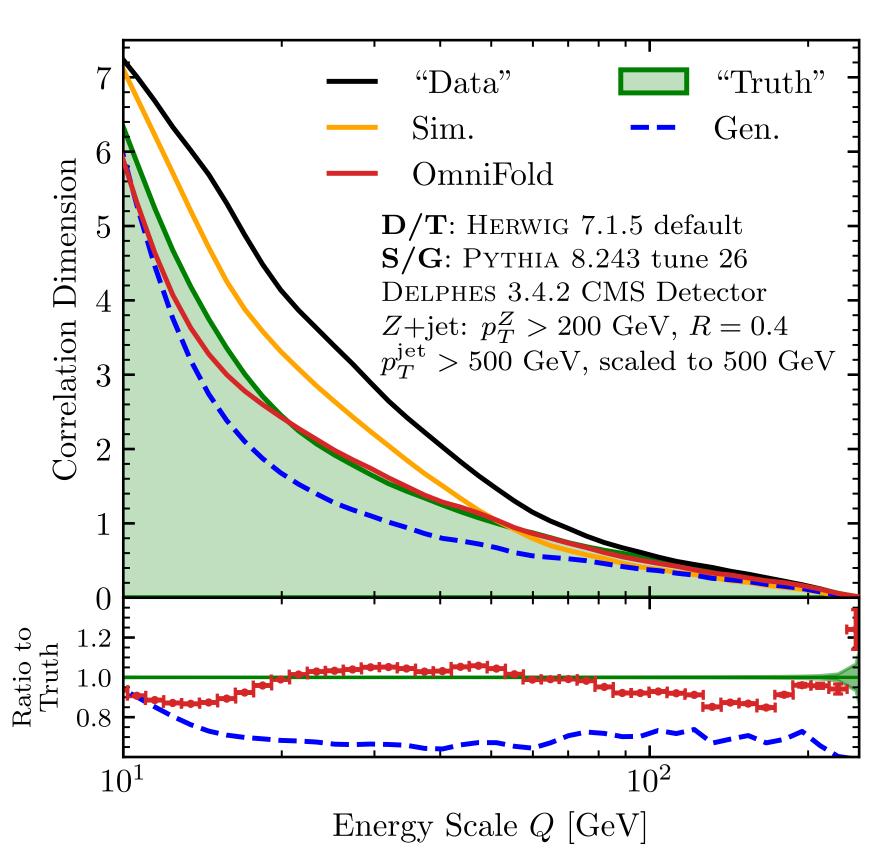


$$N_{\text{neigh.}}(Q) \propto Q^{\text{dim}} \implies \dim(Q) = Q \frac{d}{dQ} \ln N_{\text{neigh.}}(Q)$$

$$\dim(Q) = Q \frac{\partial}{\partial Q} \ln \sum_{i} \sum_{j} w_{i} w'_{j} \Theta(\text{EMD}(\mathcal{E}_{i}, \mathcal{E}'_{j}) < Q)$$

Weighted events naturally accommodated

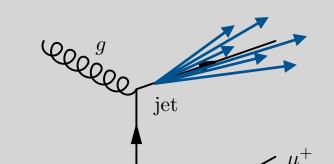


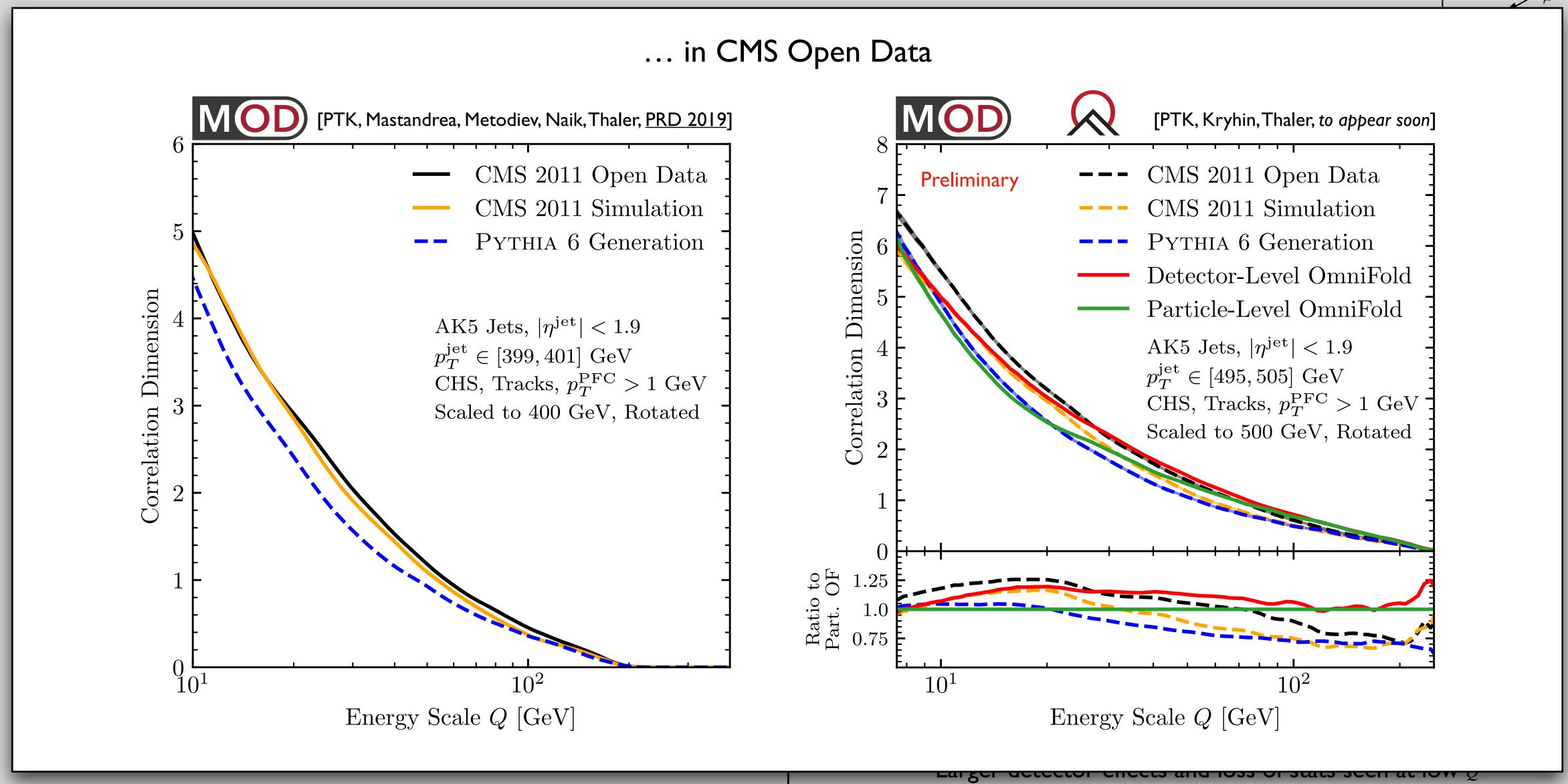


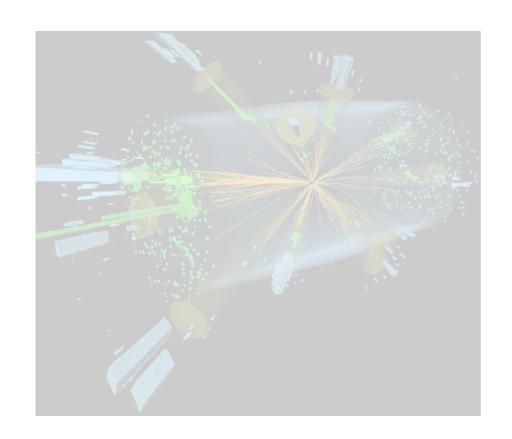
Same OmniFold training can unfold a complicated function of pairs of events!

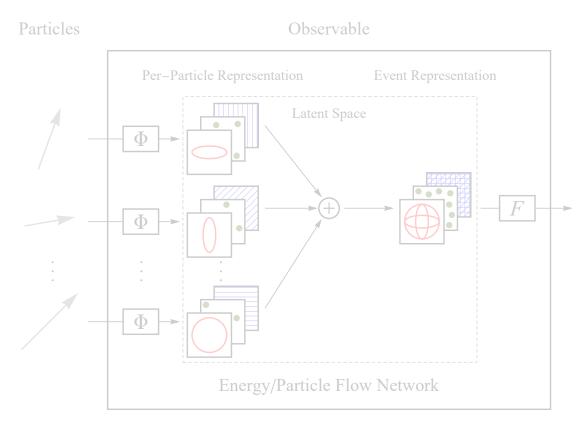
Larger detector effects and loss of stats seen at low Q

Unfolding Beyond Observables











Particle Physics Fundamentals – Jets

Jets are critical to the success of the modern collider program

Architectures for Colliders – EFNs/PFNs

Simple, extensible neural network architecture(s) for collider events

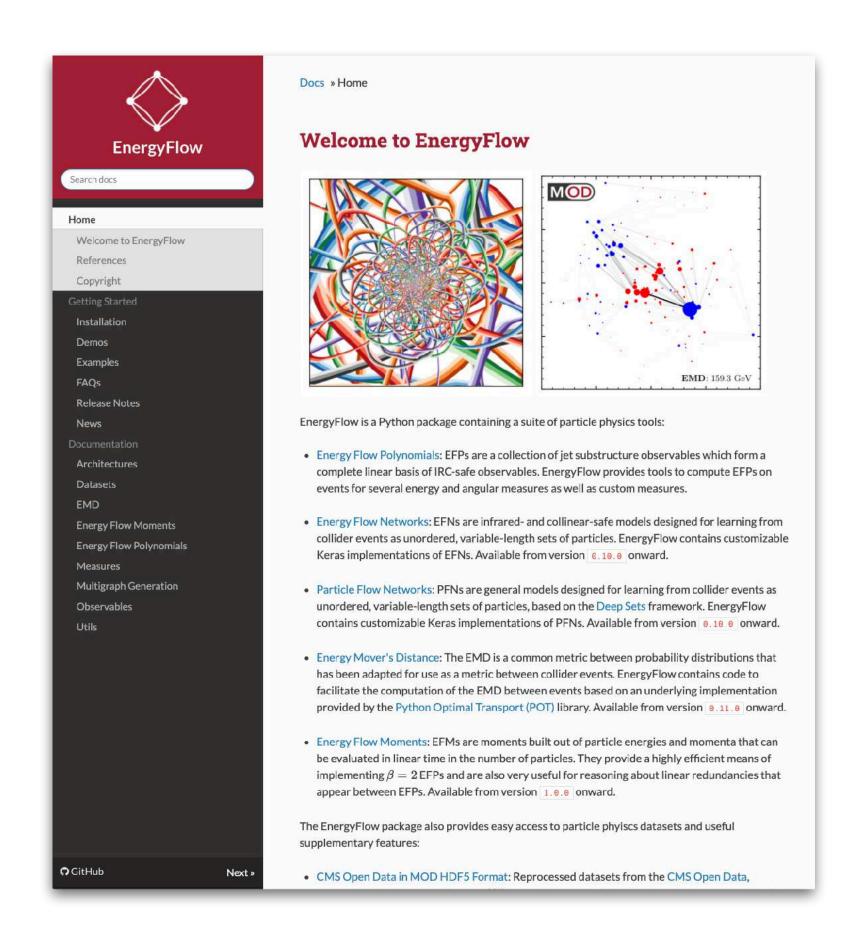
Statistical Deconvolution – OmniFold

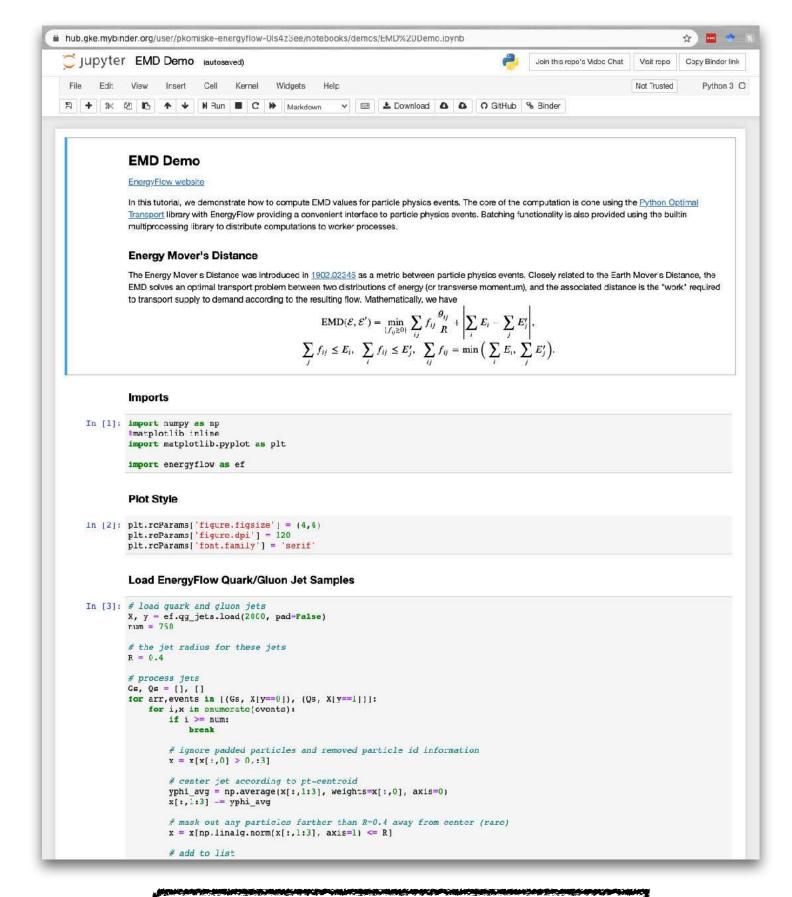
Likelihood-free inference uses high-dimensional classifiers (PFNs) to avoid explicit histograms and overcome the curse of dimensionality in unfolding

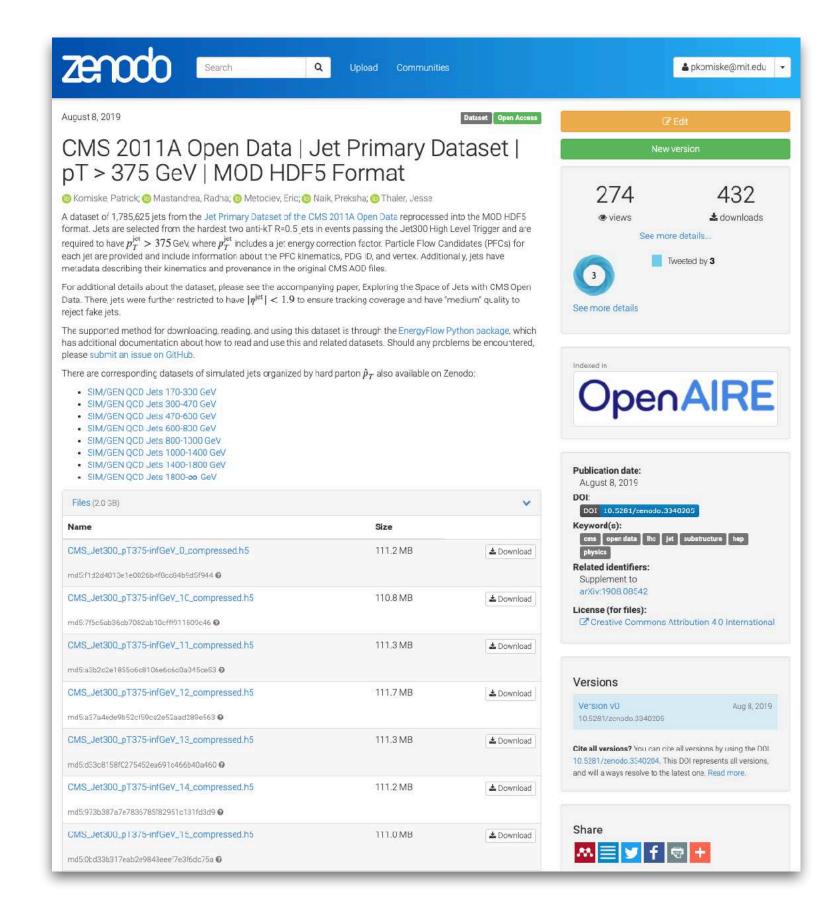
Implementations of EFNs/PFNs in Tensorflow, parallelized EMD calculations (in C++)

Detailed <u>examples</u>, <u>demos</u>, and <u>documentation</u>

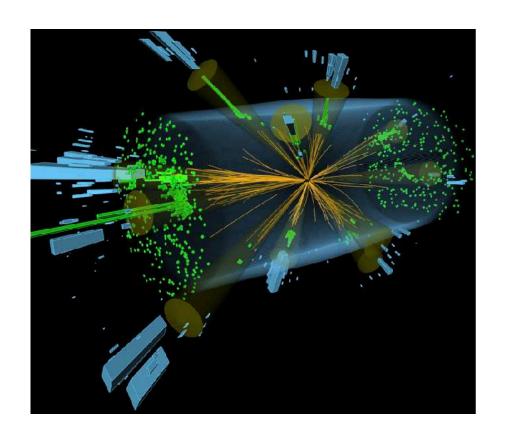
Interfaces with CMS 2011A Jet Primary Dataset (and other datasets) hosted on Zenodo

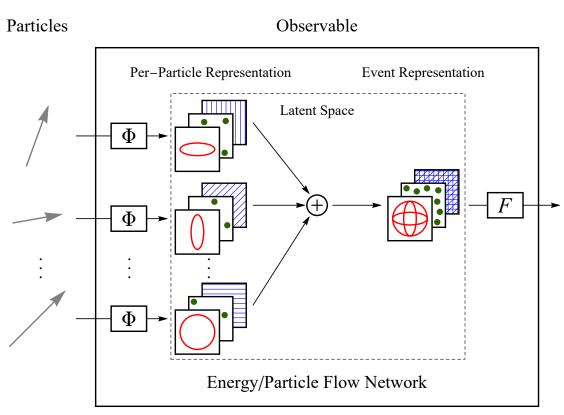






https://energyflow.network







Particle Physics Fundamentals – Jets

Jets and jet substructure will be essential to the next big collider discovery

Architectures for Colliders – EFNs/PFNs

EFNs/PFNs enable simple, fast, powerful deployment of deep learning for high-energy collider events

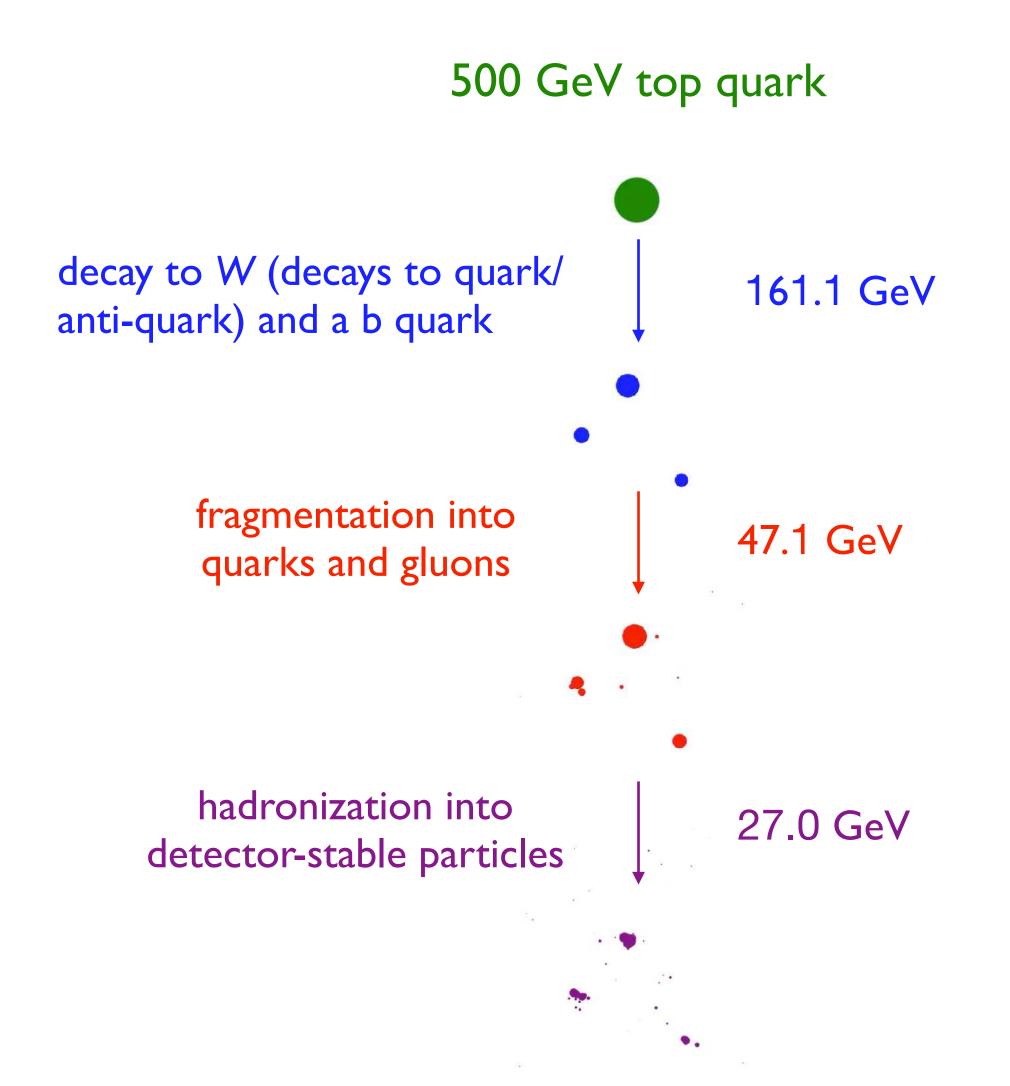
Statistical Deconvolution – OmniFold

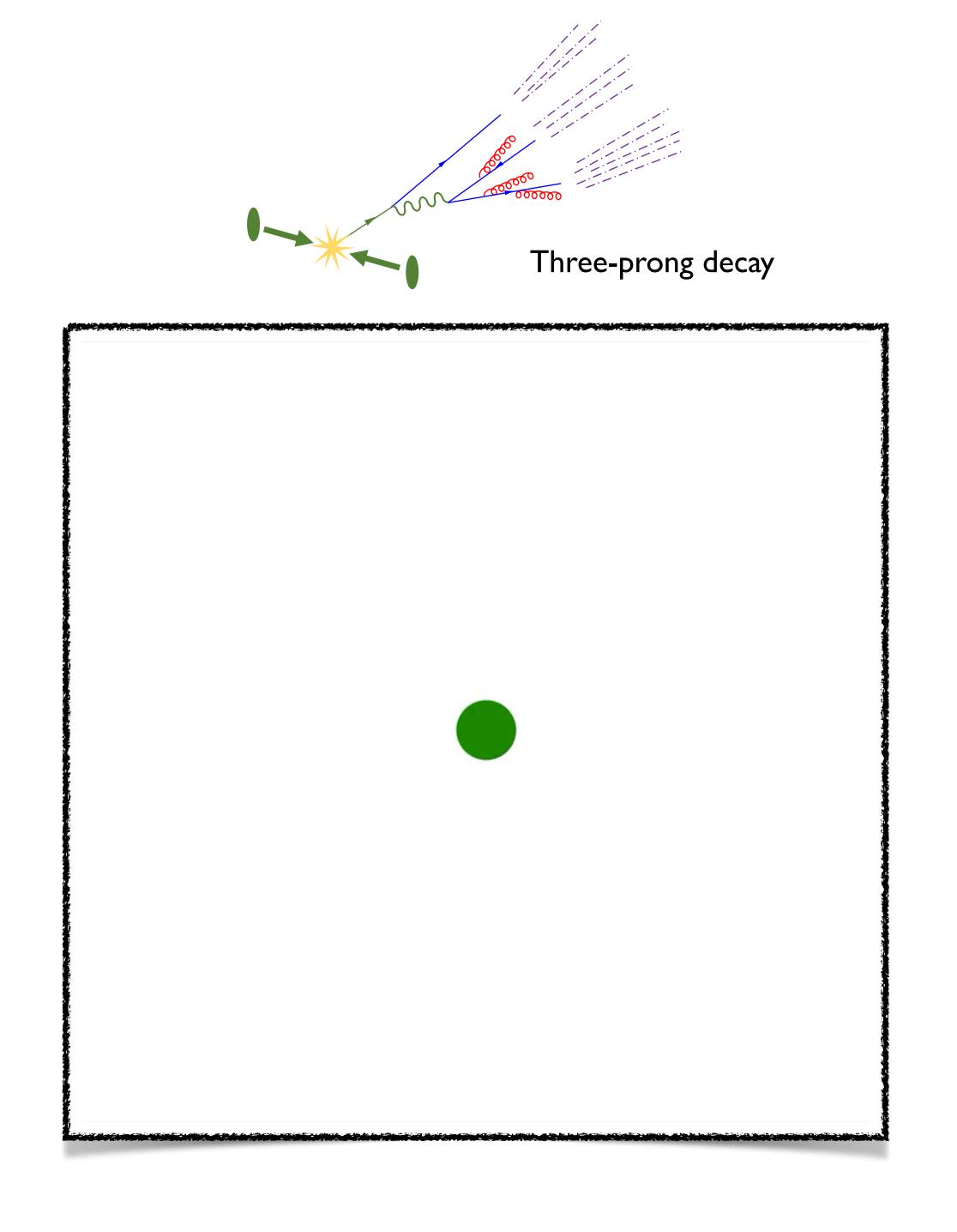
Substantially improved unfolding enables multi-differential measurements with smaller uncertainties

Thank you!

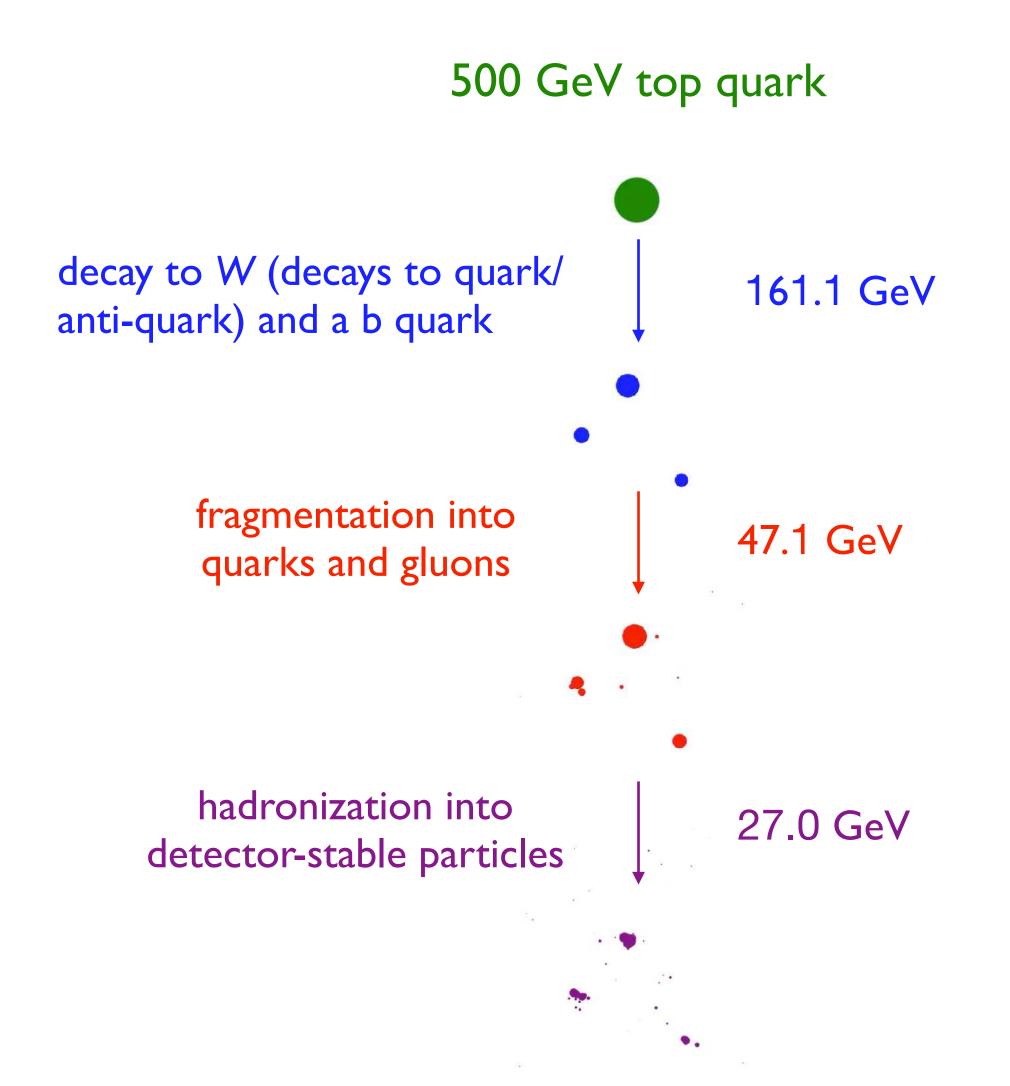
Additional Slides

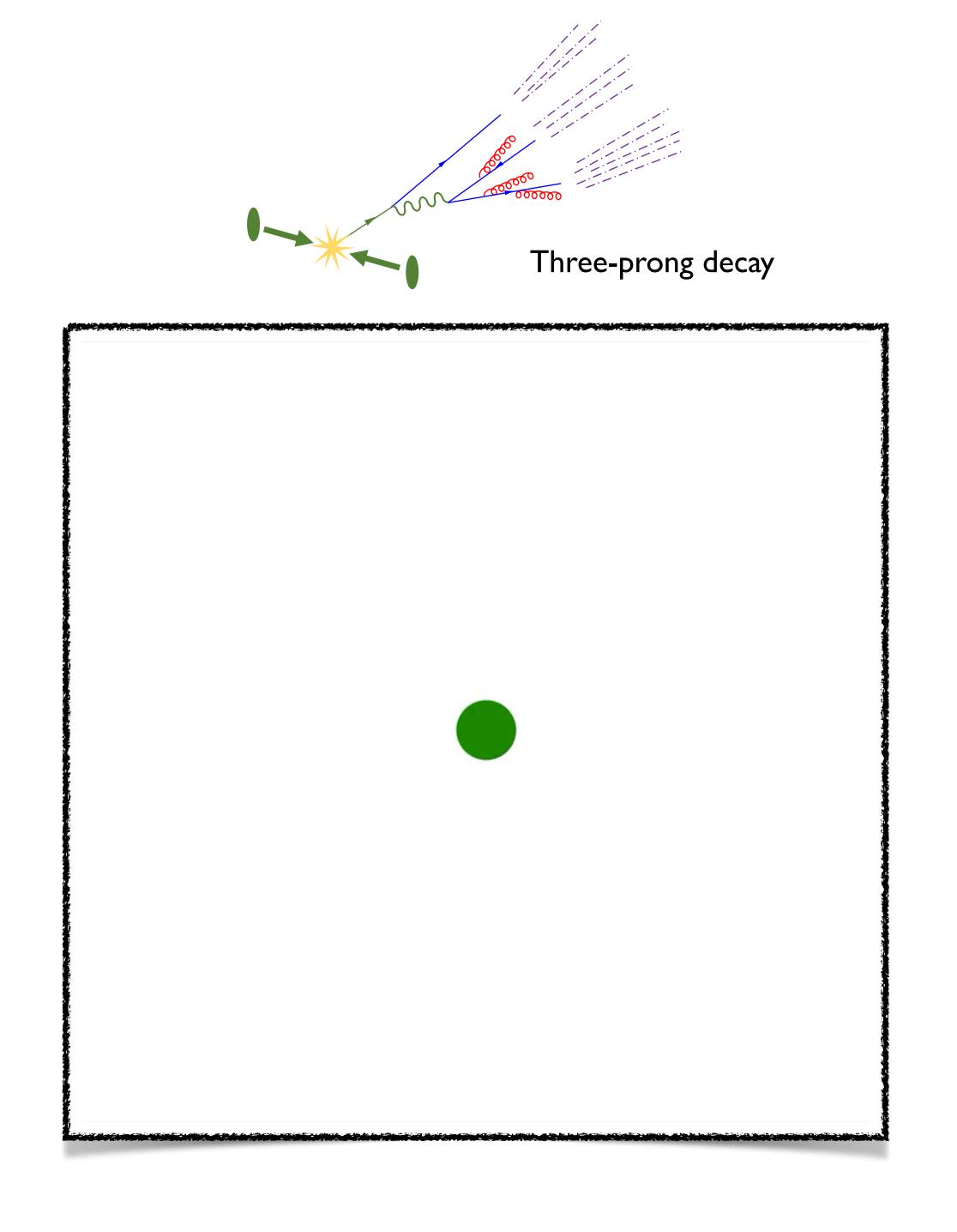
Visualizing Jet Formation – Top Jets





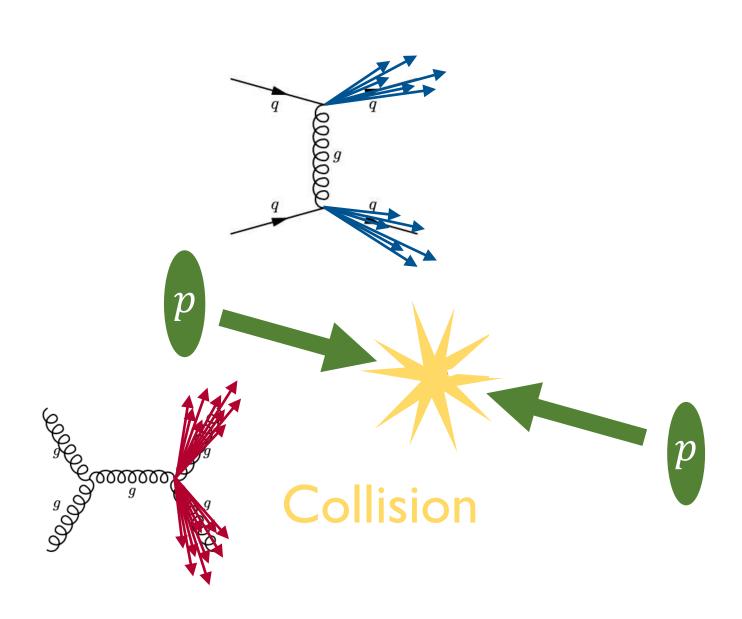
Visualizing Jet Formation – Top Jets





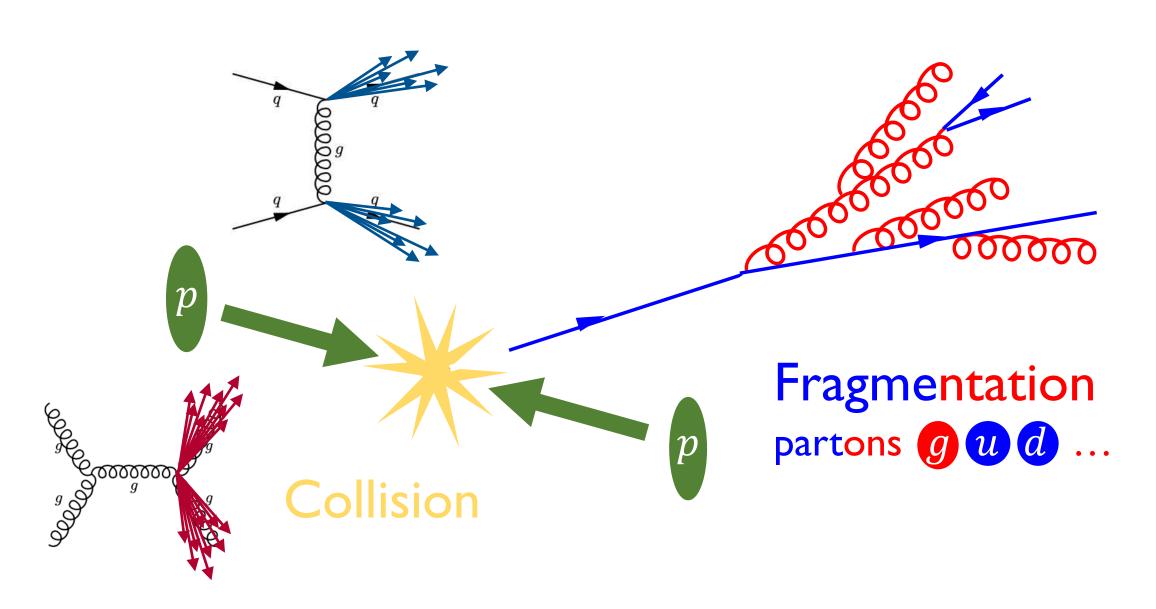
Hard collision – interesting high-energy dynamics

Perturbative quantum field theory, Feynman diagrams



Hard collision — interesting high-energy dynamics Perturbative quantum field theory, Feynman diagrams

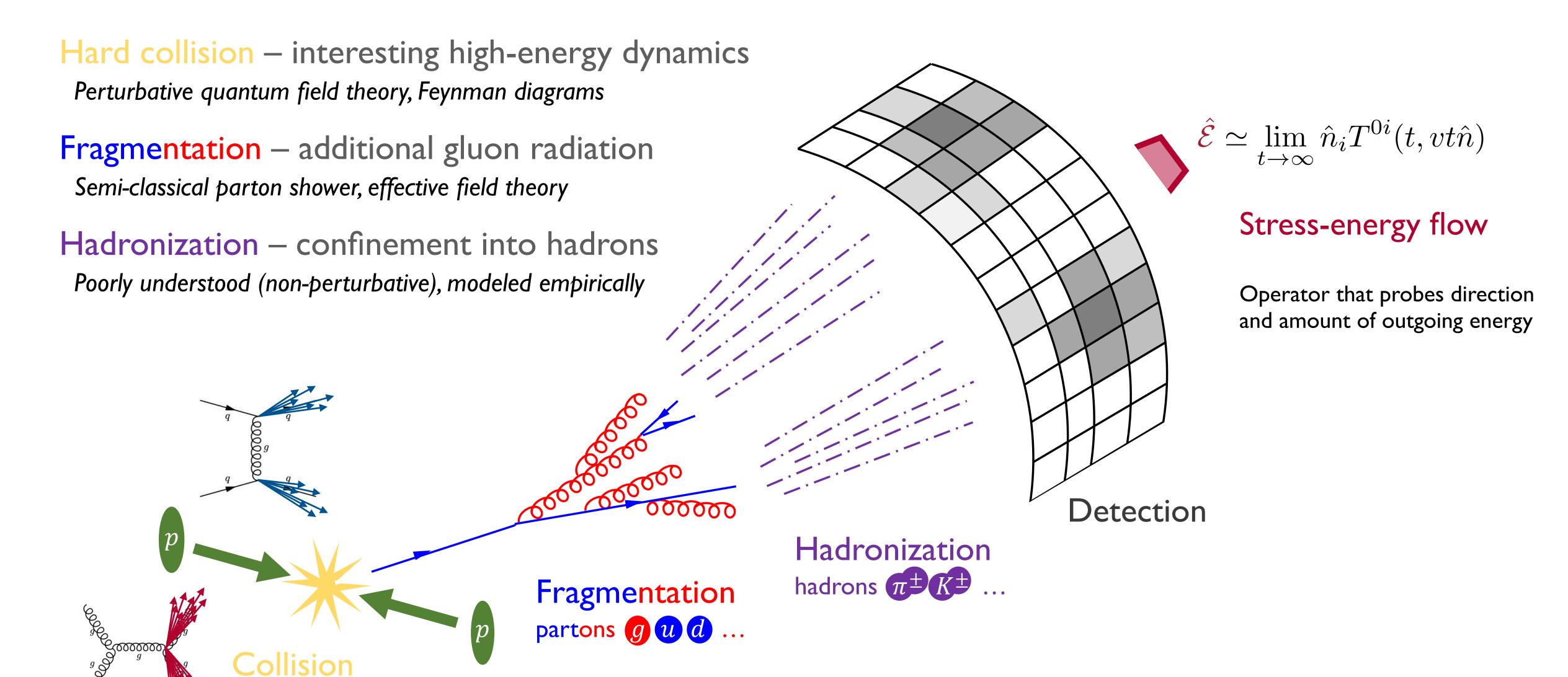
Fragmentation — additional gluon radiation
Semi-classical parton shower, effective field theory



Hard collision – interesting high-energy dynamics

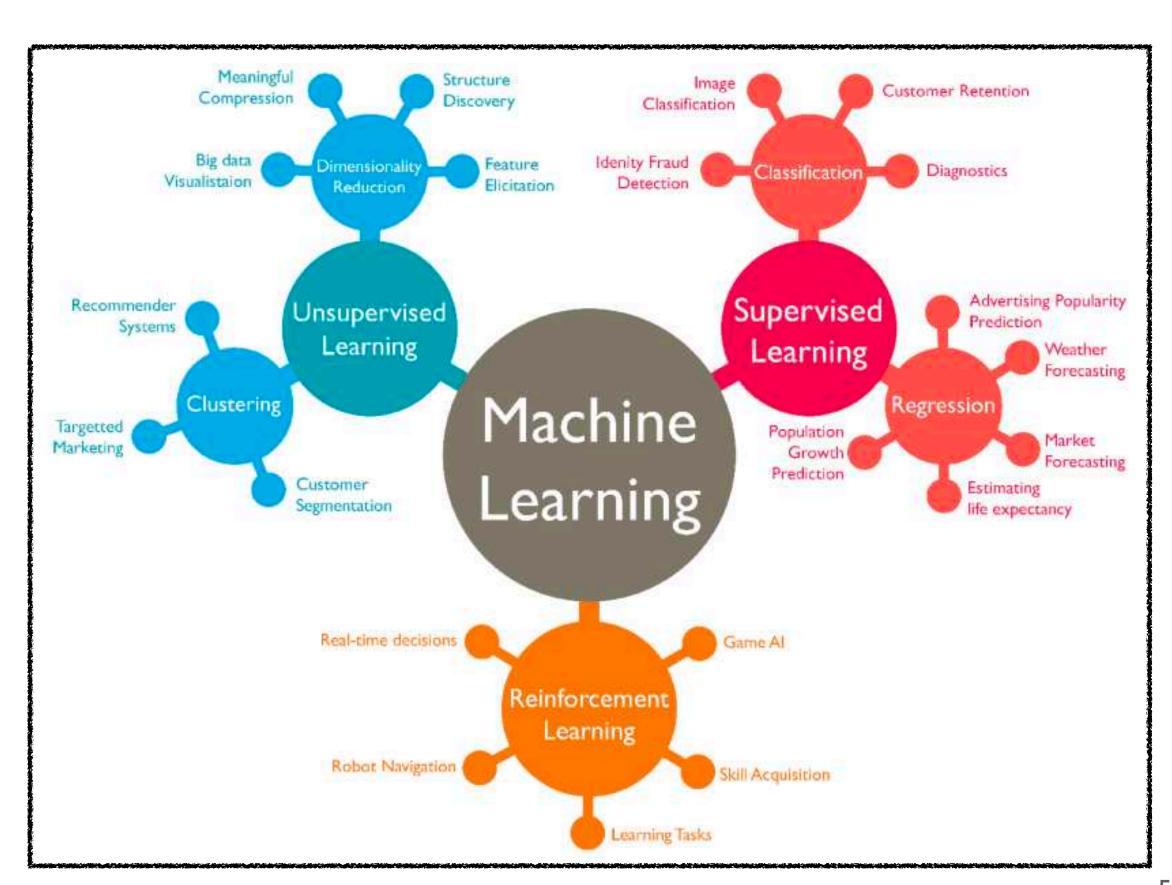
Perturbative quantum field theory, Feynman diagrams

Fragmentation – additional gluon radiation Semi-classical parton shower, effective field theory Hadronization – confinement into hadrons Poorly understood (non-perturbative), modeled empirically Hadronization hadrons $\pi^{\pm}K^{\pm}$ Fragmentation partons $gud \dots$ Collision



[Sveshnikov, Tkachov, PLB 1996; Hofman, Maldacena, JHEP 2008; Mateu, Stewart, Thaler, PRD 2013; Dixon, PTK, Moult, Thaler, Zhu, to appear soon]

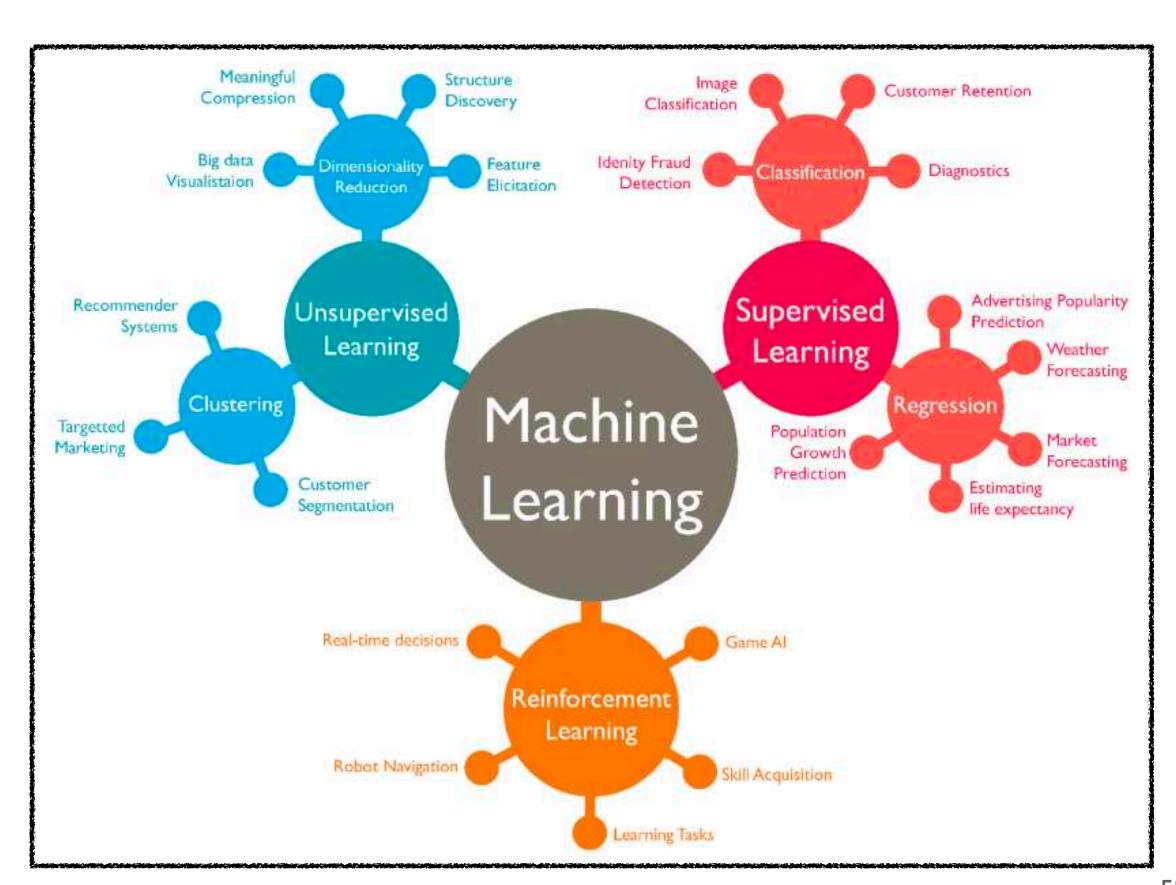
Introduction to Machine Learning



Introduction to Machine Learning

Machine learning comprises statistical algorithms and techniques designed to meaningfully engage with data

$$|\text{machine learning}\rangle \simeq |\text{data science}\rangle = \frac{|\text{statistics}\rangle + |\text{computer science}\rangle}{\sqrt{2}}$$

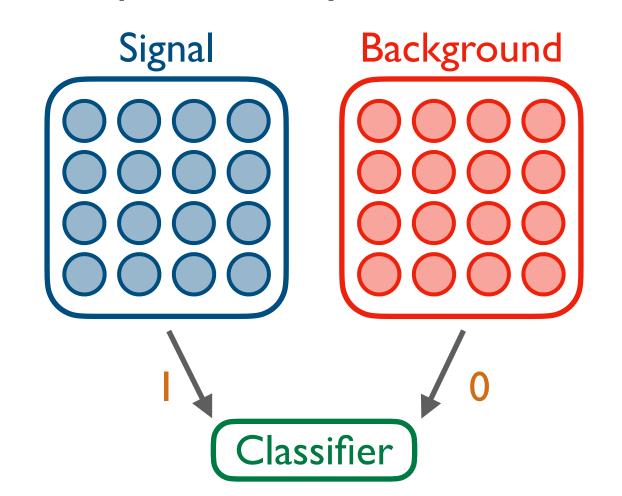


Introduction to Machine Learning

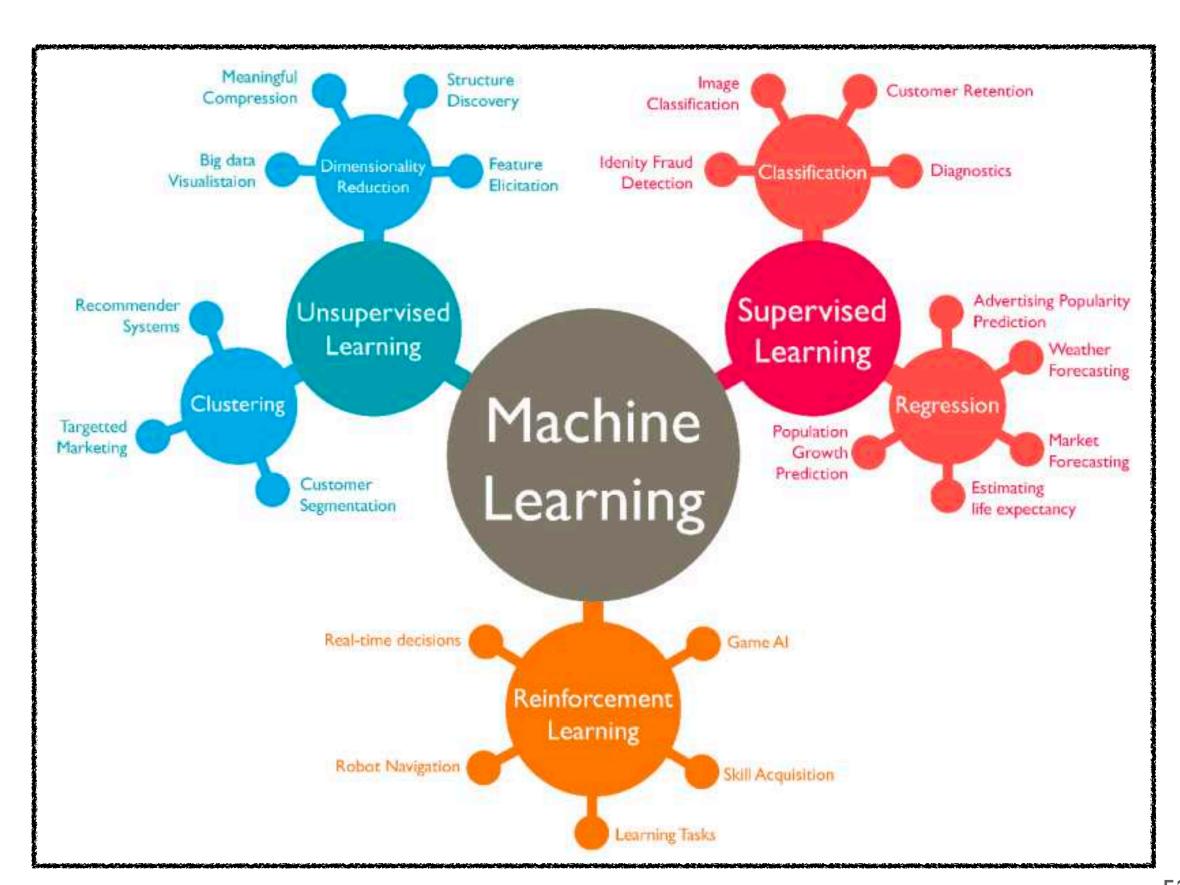
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Common paradigm – minimize a loss function $loss = \left\langle (model_{\vec{w}}(inputs) - outputs)^2 \right\rangle$



Machine Learning Considerations

The Power of ML

Automatic feature extraction

Ensures relevant features are not missed

Asymptotically optimizes performance

Provides useful/practical statistical power

Interpolation in high-dimensional spaces

Combats the curse of dimensionality

Machine Learning Considerations

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Comes at a cost

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Machine Learning Considerations – in Particle Physics

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Available data

Data source, number of samples, labels, reliability

Learning paradigm

Fully/weakly/un-supervised, classification/regression/generation



Inputs and outputs

Size/shape, symmetries, dimensionality

Model architecture

Expressibility, loss function, hyperparameters, validation/testing



Model implementation, training/evaluation speed, uncertainties



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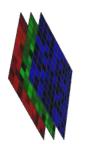


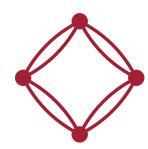
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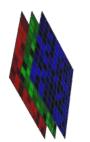


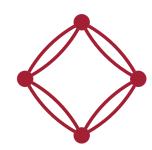
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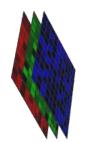


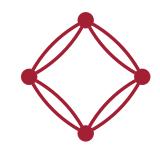
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Deployment strategy





Thoughts on Machine Learning

Machine learning will be essential in maximizing HEP potential

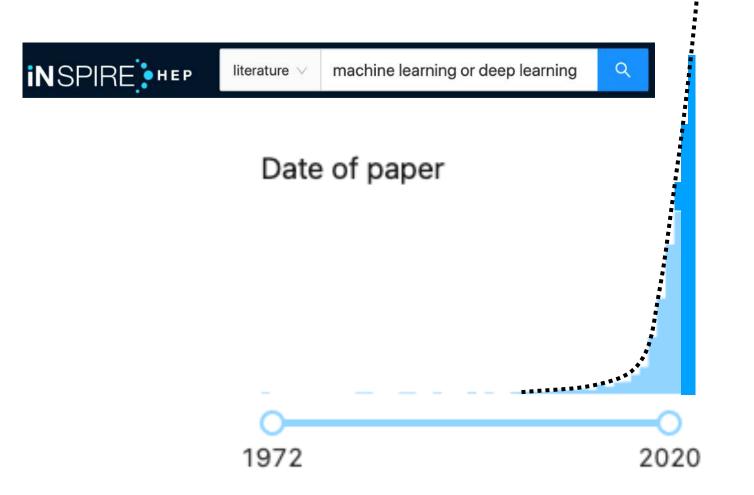
We should capitalize on the opportunity to optimize ML is both a computational tool and a useful formalism/language

High-energy physics can benefit ML

e.g. EFNs are weighted deep sets, EFN2/PFN2 will have broader applications NSF Institute for Artificial Intelligence and Fundamental Interactions

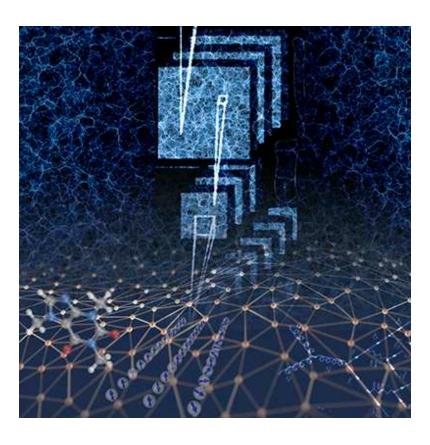
Collaboration across traditional lines will enable success
 Theorists, experimentalists, and ML experts all can and should contribute

Computational best practices can be shared among fields
 Software workflows, reproducible analyses, public datasets are critical



HEPML-LivingReview has a thorough and organized list of papers

$$(\{p_i^{\mu}\}) = F\left(\underbrace{\sum_{i} z_i \Phi^{(\ell_1)}(\hat{p}_i)}_{\Phi_1}, \underbrace{\sum_{i} \sum_{j} z_i z_j \Phi^{(\ell_2)}(\hat{p}_i, \hat{p}_j)}_{\Phi_2}, \dots\right)$$



[Reviews of Modern Physics Cover December 2019 from Machine learning and the physical sciences]

Future Development of Architectures, Algorithms, and Techniques

Beyond single-particle point cloud architectures

Pairwise information known to be physically meaningful "EFN2/PFN2" has greater expressivity for tagging and unfolding

► EMD-inspired techniques for theory and experiment

New and better grooming and pileup mitigation techniques for LHC and beyond Bootstrap "event space" to "theory space"

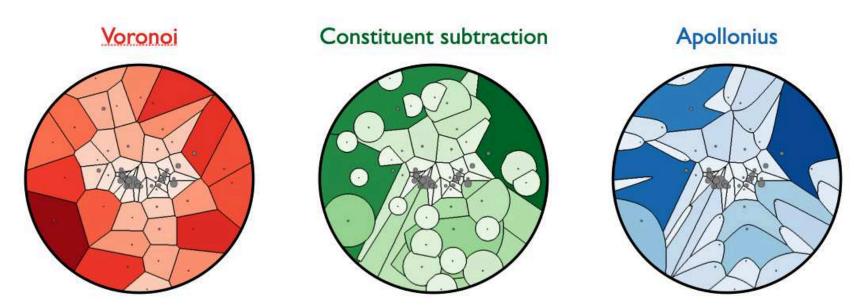
Public datasets provide rich context for testing new methods

Novel search strategies can be tried directly (e.g. dimuon resonances with pT cut)

Data preservation critical for maximizing scientific benefit (e.g. ALEPH e+e- data)

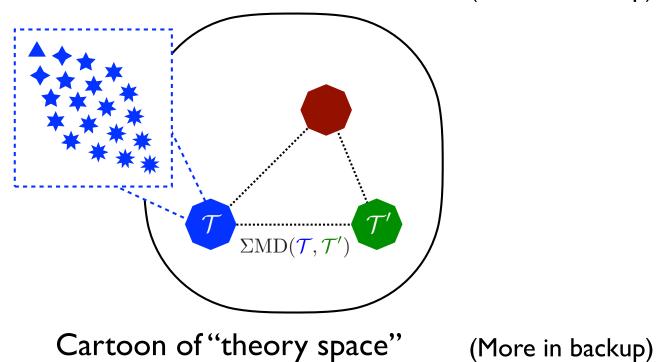
Opportunities pursue novel investigation strategies in HEP

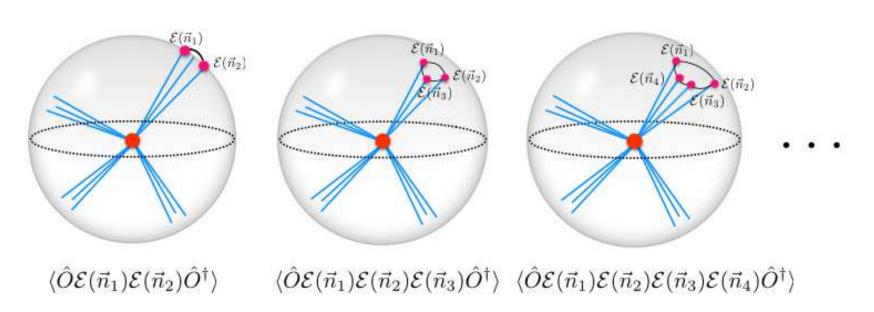
Weighted cross sections probe physics differently than traditional observables e.g. energy-energy correlators, which utilize CFT techniques for QCD calculations



Pileup subtraction methods on example jet from CMS Open Data

(More in backup)

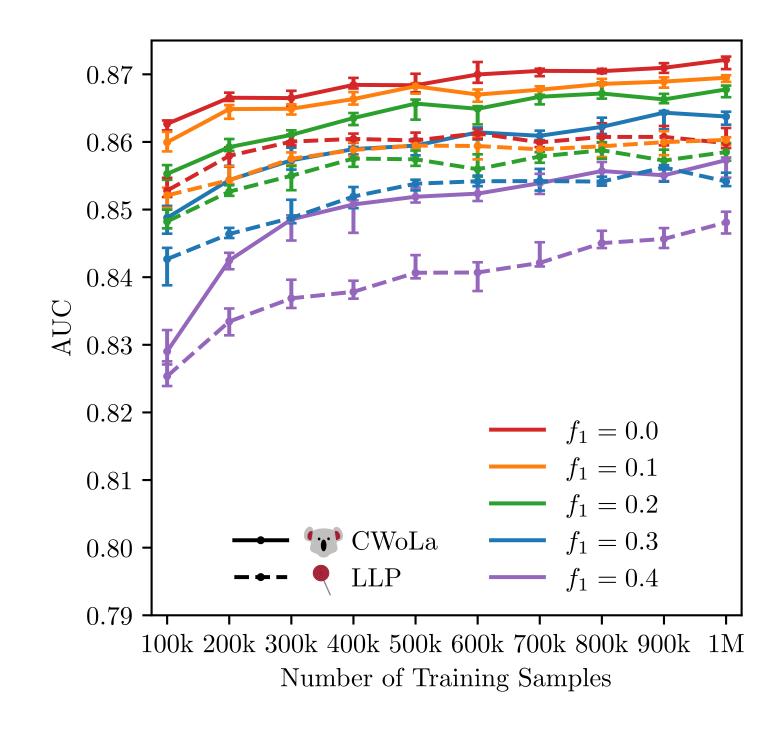




Correlations of energy flow operators on celestial sphere (More in <u>backup</u>)

Training On Data

[Metodiev, Nachman, Thaler, JHEP 2017; PTK, Metodiev, Nachman, Schwartz, PRD 2018; Metodiev, Thaler, PRL 2018; PTK, Metodiev, Thaler, JHEP 2018]



Gluon Jet Background Rejection
0.0
7.0
8.0
8.0 **EFPs: Extracted ROCs** Рутнія 8.230, $\sqrt{s} = 14 \text{ TeV}$ $R = 0.4, p_T \in [500, 550] \text{ GeV}$ Truth EFPs Extracted CNN Extracted Soft Drop Multiplicity $n_{\rm SD}$ Extracted N-subjettiness $\tau_2^{(\beta=1)}$ Extracted Jet Mass m Extracted 0.0 +0.20.8 0.00.40.6Quark Jet Signal Efficiency

35.9 fb⁻¹ (13 TeV) CMS Multijet Data Events 10⁷ ttcc tt2b Small bkgs Stat uncert 10⁴ 10^{3} 0.2 0.6 **CWoLa BDT**

CWoLa can be used to train high-dimensional classifiers on mixed samples without labels

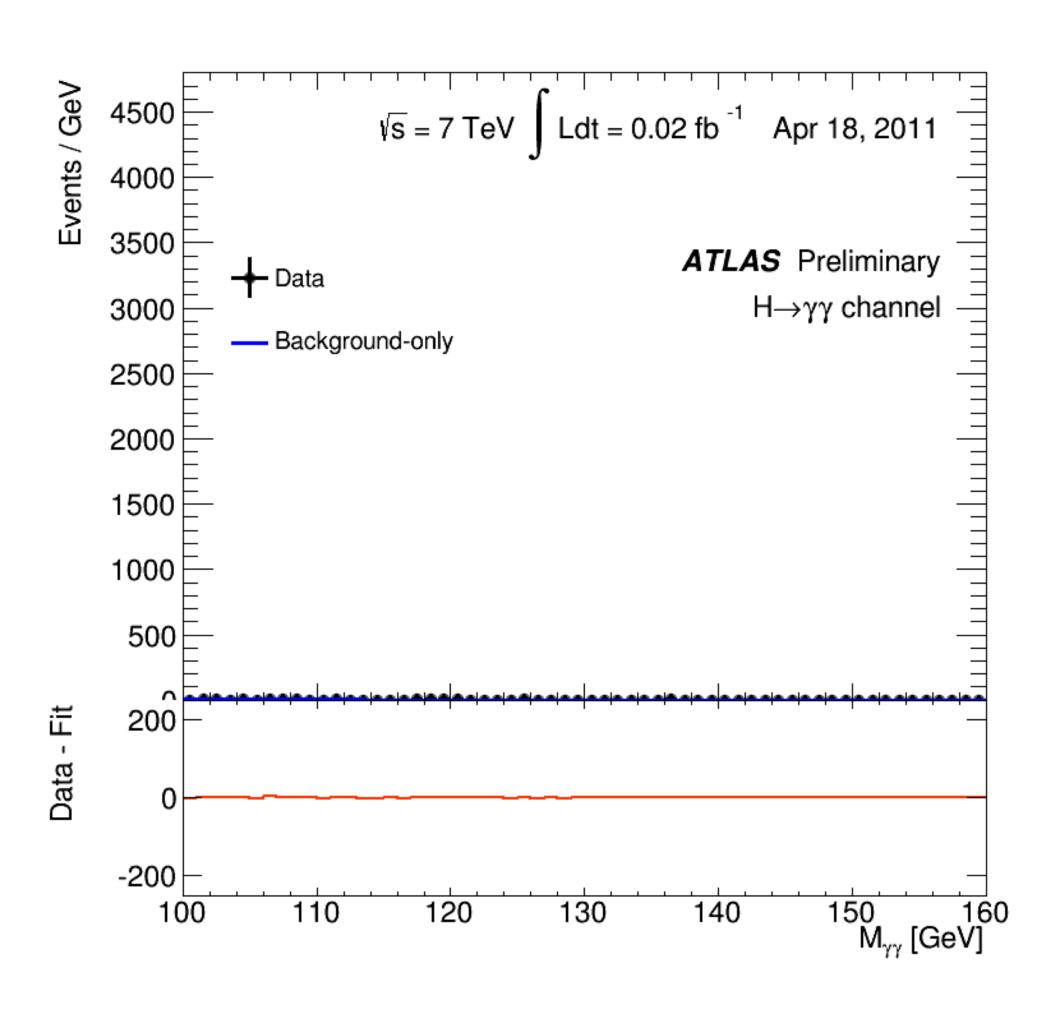
Classifiers can be calibrated with topic modeling

CWoLa used to train BDT in CMS data

[CMS, PLB 2020]

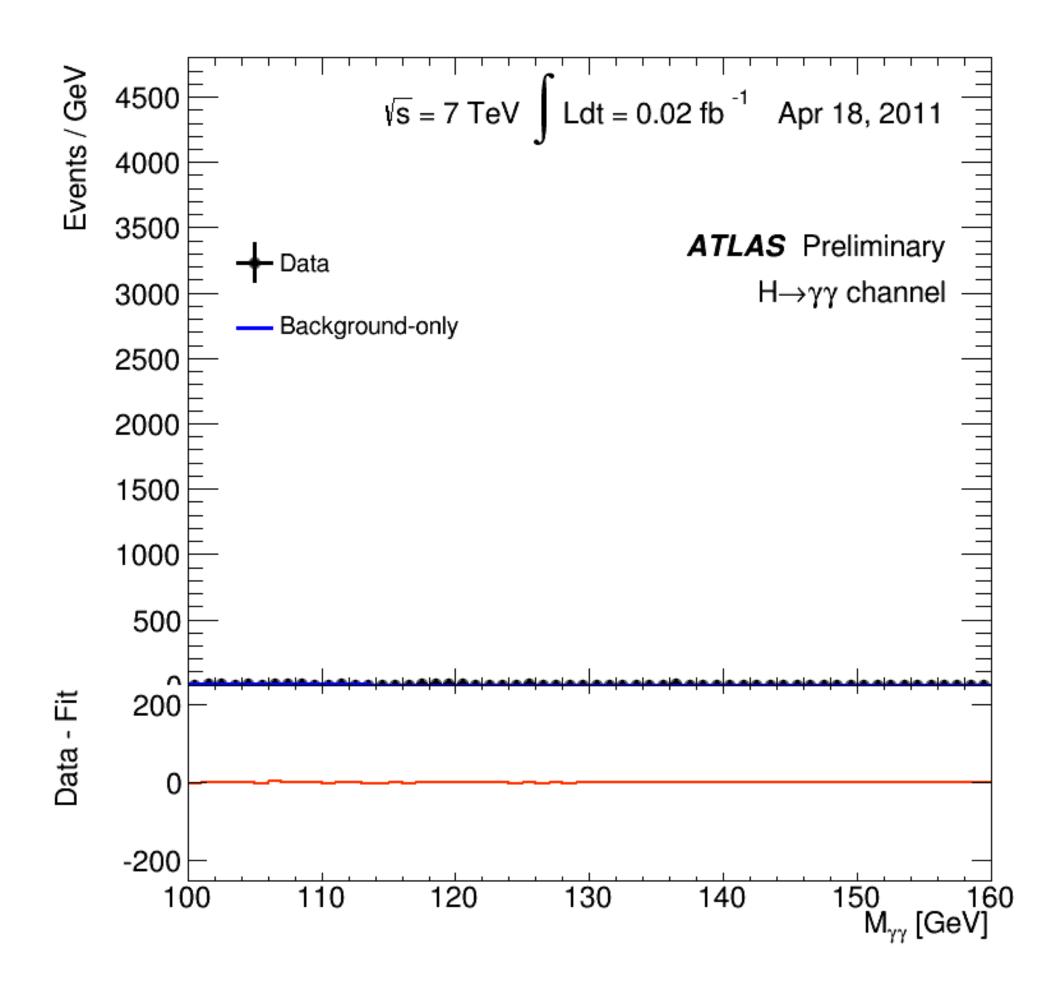
Statistical Ensembles of Events

Histograms show the distribution of events according to some particular feature



Statistical Ensembles of Events

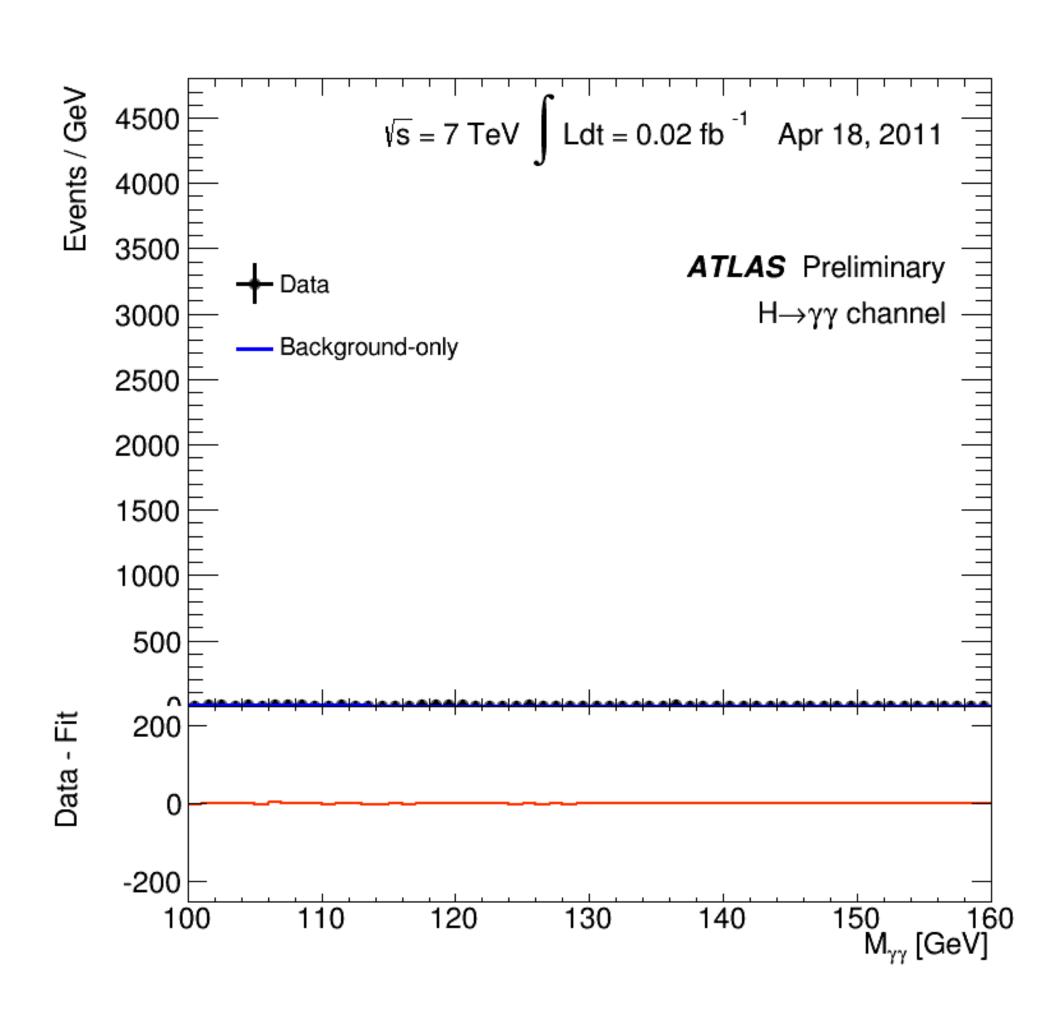
Histograms show the distribution of events according to some particular feature



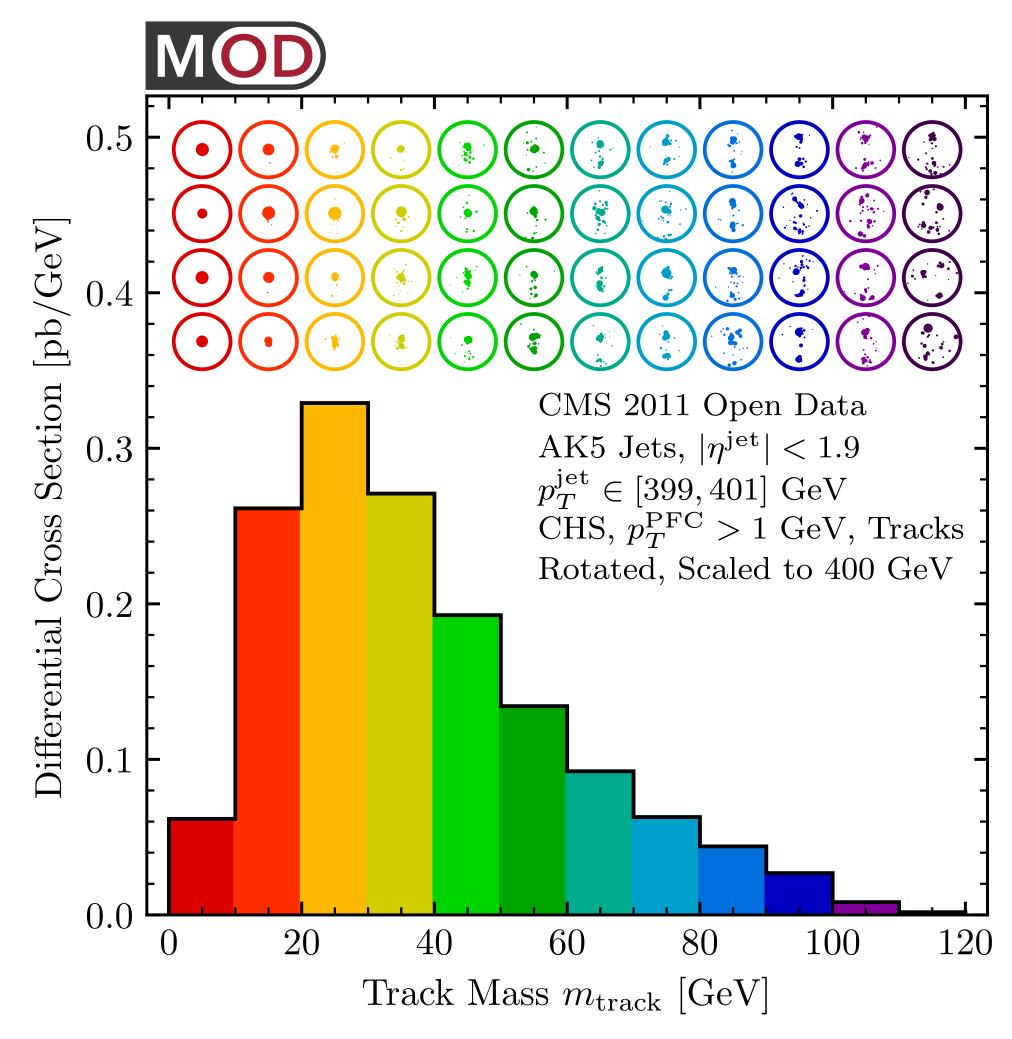
Discovering the Higgs boson from two photons

Statistical Ensembles of Events

Histograms show the distribution of events according to some particular feature



Discovering the Higgs boson from two photons



Showing events by the combined "mass" of their charged particles

Infrared and Collinear (IRC) Safety

QCD has soft and collinear divergences associated with gluon radiation

$$dP_{i \to ig} \simeq \frac{2\alpha_s}{\pi} C_a \frac{d\theta}{\theta} \frac{dz}{z} \qquad C_q = C_F = 4/3$$

$$C_g = C_A = 3$$

Infrared (IR) safety – observable is unchanged by adding a soft particle

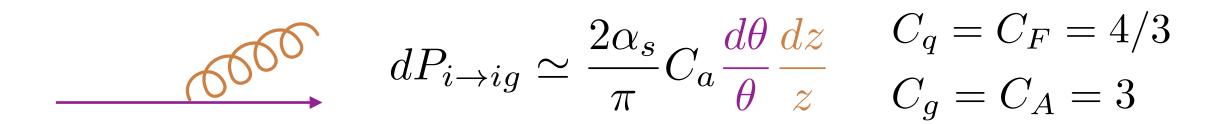
Collinear (C) safety – observable is unchanged by a collinear splitting

$$= \underbrace{\epsilon \to 0}_{}$$

$$= \underbrace{1 - \lambda \quad \lambda}_{}$$

[PTK, Metodiev, Thaler, JHEP 2020]

QCD has soft and collinear divergences associated with gluon radiation



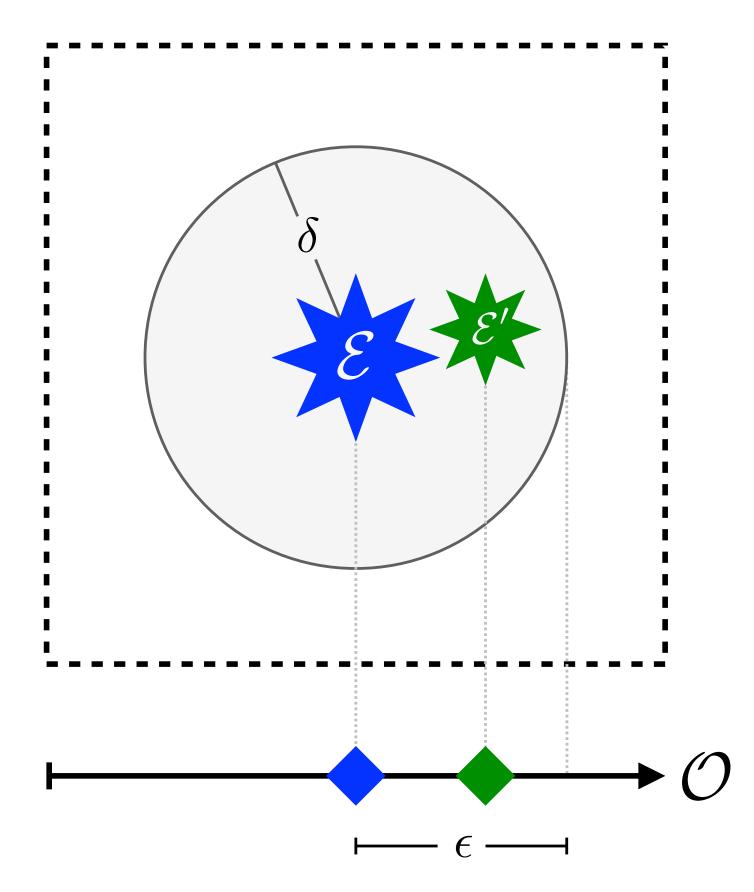
Infrared (IR) safety – observable is unchanged by adding a soft particle

Collinear (C) safety – observable is unchanged by a collinear splitting

$$= \underbrace{\hspace{1cm}}^{\epsilon \to 0} = \underbrace{\hspace{1cm}}^{1 - \lambda} \lambda$$

*on all but a negligible set‡ of events

‡a negligible set is one that contains no positive-radius EMD-ball



Classic $\epsilon - \delta$ definition of continuity in metric topology

An observable \mathcal{O} is EMD continuous at an event \mathcal{E} if, for any $\epsilon > 0$, there exists a $\delta > 0$ such that for all events \mathcal{E}' :

$$\mathrm{EMD}(\mathcal{E},\mathcal{E}') < \delta \implies |\mathcal{O}(\mathcal{E}) - \mathcal{O}(\mathcal{E}')| < \epsilon.$$

Energy Flow Methods

Energy Flow Polynomials (EFPs)

[PTK, Metodiev, Thaler, JHEP 2018]

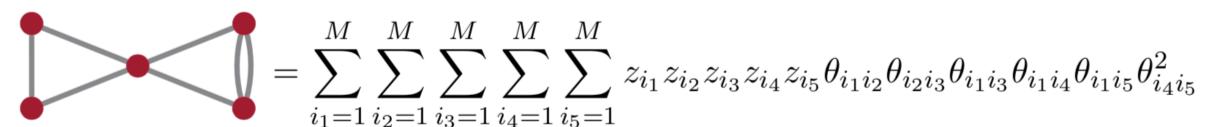
Obtained via systematically expanding in energies and angles

EFPs are multiparticle correlators

$$\sum_{i_1=1}^{M} \cdots \sum_{i_N=1}^{M} z_{i_1} \cdots z_{i_N} \prod_{(j,k) \in G} \theta_{i_j i_k}^{\beta}$$



e.g.



Any IRC-safe observable S is a linear combination of EFPs!

$$\mathcal{S} \simeq \sum_{G \in \mathcal{G}} s_G \mathrm{EFP}_G$$
, \mathcal{G} a set of multigraphs

Definition of energy factor and pairwise angular distance

$$pp: z_i = \frac{p_{Ti}}{\sum_j p_{Tj}} \qquad \theta_{ij}^2 = 2n_i^{\mu} n_{j\mu} = 2\frac{p_i^{\mu}}{p_{Ti}} \frac{p_{\mu j}}{p_{Tj}} \simeq (y_i - y_j)^2 + (\phi_i - \phi_j)^2$$

$$\mathbf{e^+e^-}$$
: $\mathbf{z_i} = \frac{E_i}{\sum_j E_j}$ $\theta_{ij}^2 = 2n_i^{\mu}n_{j\mu} = 2\frac{p_i^{\mu}}{E_i}\frac{p_{j\mu}}{E_j}$

Organized by number of edges d

Degree	Connected Multigraphs		
d = 0	•		
d = 1			
d=2			
d = 3			
d = 4			
d = 5			

Energy Flow Moments (EFMs)

$$\theta_{ij} = \sqrt{2n_i^{\mu}n_{j\mu}}$$
 $\beta = 2$ removes square root

Factors of n_i^{μ} can be organized in optimal way

 EFM_v is a little group tensor with v indices

$$\mathcal{I}^{\mu_1\cdots\mu_v} = \sum_{i=1}^M z_i n_i^{\mu_1} \cdots n_i^{\mu_v}$$

$$\mathcal{I}^{j_1 j_2 \cdots j_v} = 2^{v/2} \Theta^{j_1 j_2 \cdots j_v}$$

spatial e⁺e⁻ EFMs

linearized sphericity tensors [Donoghue, Low, Pi, PRD 1979]

$$= \sum_{i_{1}=1}^{M} \sum_{i_{2}=1}^{M} \sum_{i_{3}=1}^{M} z_{i_{1}} z_{i_{2}} z_{i_{3}} \theta_{i_{1}i_{2}}^{2} \theta_{i_{1}i_{3}}^{2} \theta_{i_{2}i_{3}}$$

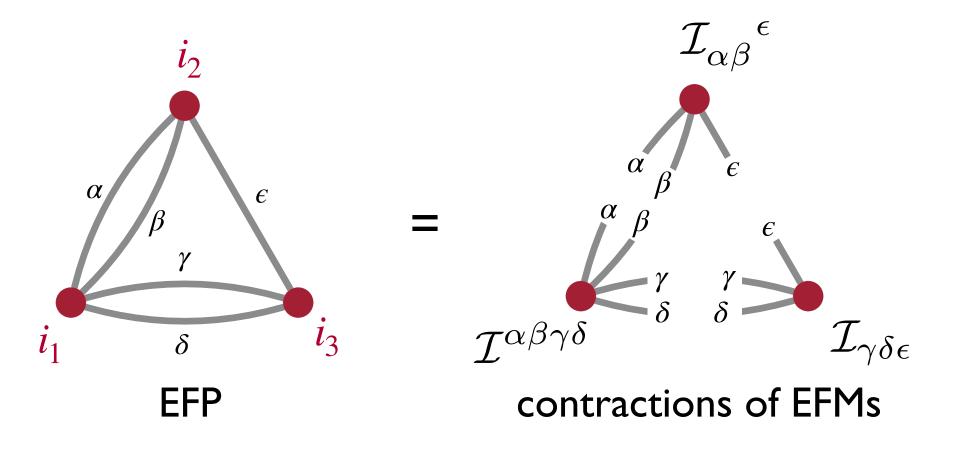
$$= 2^{5} \underbrace{\left(\sum_{i_{1}=1}^{M} z_{i_{1}} n_{i_{1}}^{\alpha} n_{i_{1}}^{\beta} n_{i_{1}}^{\gamma} n_{i_{1}}^{\delta}\right)}_{\mathcal{I}_{\alpha\beta}^{\beta\gamma\delta}} \underbrace{\left(\sum_{i_{2}=1}^{M} z_{i_{2}} n_{i_{2}\alpha} n_{i_{2}\beta} n_{i_{2}}^{\epsilon}\right)}_{\mathcal{I}_{\alpha\beta}^{\epsilon}} \underbrace{\left(\sum_{i_{3}=1}^{M} z_{i_{3}} n_{i_{3}\gamma} n_{i_{3}\delta} n_{i_{3}\epsilon}\right)}_{\mathcal{I}_{\gamma\delta\epsilon}}$$

Naively $\mathcal{O}(M^3)$ EFP shown to be $\mathcal{O}(M)$

All $\beta = 2$ EFPs are $\mathcal{O}(M)$

- $\mathrm{ECF}_{N}^{(\beta=2)}$ are all $\mathcal{O}(M)$ $D_{2}^{(\beta=2)}$, $C_{2}^{(\beta=2)}$ are $\mathcal{O}(M)$

EFMs result from cutting edges of EFP



(See backup for more on understanding linear redundancies and counting superstring amplitudes with EFMs)

Understanding Linear Redundancies via EFMs

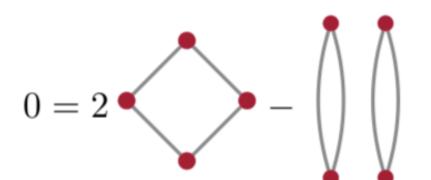
[PTK, Metodiev, Thaler, PRD 2020]

Linear redundancies among EFPs are troublesome

Studying coefficients of linear fit difficult $\mathcal{O} = \sum_G s_G \mathrm{EFP}_G$

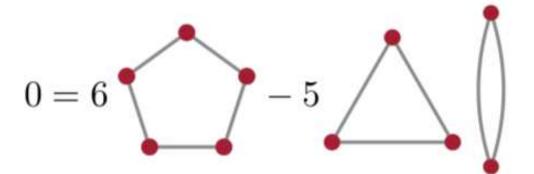
Examples of redundancies

in 3 or fewer spacetime dimensions

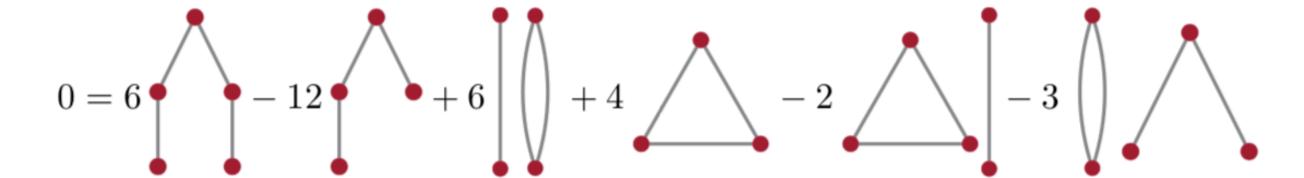


$$0 = \mathcal{I}^{\beta}_{[\alpha} \mathcal{I}^{\gamma}_{\beta} \mathcal{I}^{\delta}_{\gamma} \mathcal{I}^{\alpha}_{\delta]}$$

in 4 or fewer spacetime dimensions



$$0 = \mathcal{I}^{\beta}_{[\alpha} \mathcal{I}^{\gamma}_{\beta} \mathcal{I}^{\delta}_{\gamma} \mathcal{I}^{\epsilon}_{\delta} \mathcal{I}^{\alpha}_{\epsilon]}$$



How to obtain a tensor identity

Consider tensor over *n* dimensional vector space

Antisymmetrize m > n indices

Result is zero because any assignment of n possible values to m slots has a repetition

$$T_{b_1\cdots b_\ell[c_1\cdots c_m]}^{a_1\cdots a_k} = 0$$

Bonus: all tensor identities up to ones governed by existing symmetries take above form

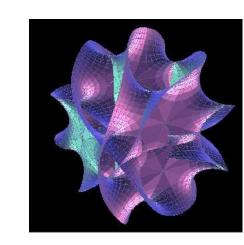
[Sneddon, Journal of Mathematical Physics]

In e⁺e⁻ there are additional relations due to

$$n_i^{\mu} = (1, \hat{n})^{\mu} \implies \mathcal{I}^{0\mu_1\cdots\mu_v} = \sqrt{2}\mathcal{I}^{\mu_1\cdots\mu_v}$$

See backup for more on these "Euclidean" relations

Counting Superstring Amplitudes



Constructing a basis of amplitudes – how large is it?

[Boels, <u>1304.7918</u>; OEIS <u>A226919</u>]

non-isomorphic multigraph



Q:What is the number of symmetric polynomials of degree d in kinematic variables up to momentum conservation?

A: Same as the number of non-isomorphic multigraphs with no leaves (vertices of valency one)

New OEIS Entries! <u>A307317, A307316</u>

Leafless Multigraphs			
	Connected	All	
Edges d	A307317	A307316	
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	$\mathbf{2553}$	3129	
11	$\mathbf{9574}$	11458	
12	$\boldsymbol{38005}$	$\mathbf{44576}$	
13	157306	181071	
14	679682	770237	
15	3047699	3407332	
16	14150278	15641159	
CONTROL OF THE PARTY OF THE PAR			

Bolded values previously unknown

Machine Learning for Point Clouds – Deep Sets

A general permutation-symmetric function is additive in a latent space

Deep Sets

[<u>1703.06114</u>]

Manzil Zaheer^{1,2}, Satwik Kottur¹, Siamak Ravanbhakhsh¹, Barnabás Póczos¹, Ruslan Salakhutdinov¹, Alexander J Smola^{1,2}

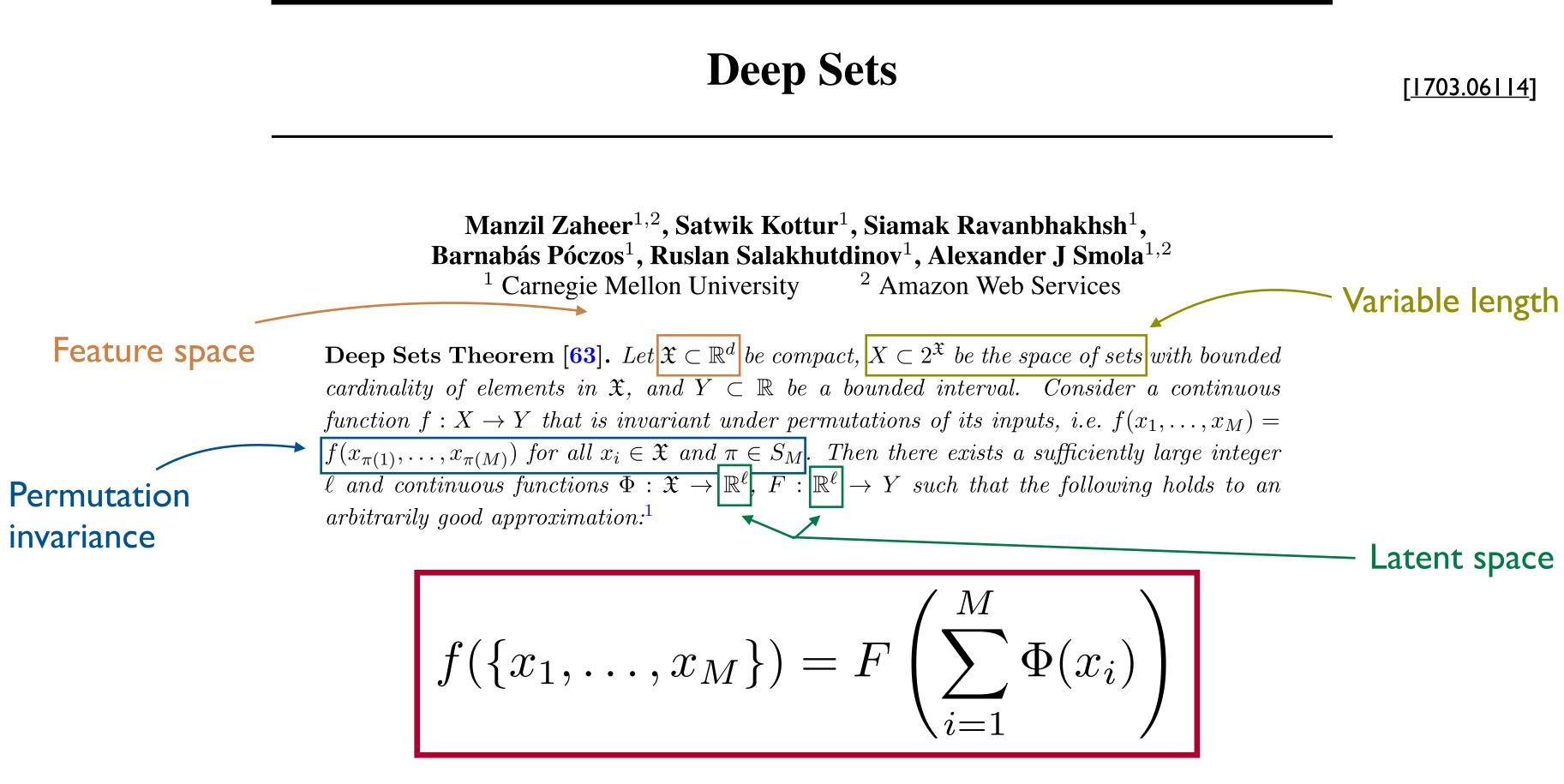
¹ Carnegie Mellon University ² Amazon Web Services

Deep Sets Theorem [63]. Let $\mathfrak{X} \subset \mathbb{R}^d$ be compact, $X \subset 2^{\mathfrak{X}}$ be the space of sets with bounded cardinality of elements in \mathfrak{X} , and $Y \subset \mathbb{R}$ be a bounded interval. Consider a continuous function $f: X \to Y$ that is invariant under permutations of its inputs, i.e. $f(x_1, \ldots, x_M) = f(x_{\pi(1)}, \ldots, x_{\pi(M)})$ for all $x_i \in \mathfrak{X}$ and $\pi \in S_M$. Then there exists a sufficiently large integer ℓ and continuous functions $\Phi: \mathfrak{X} \to \mathbb{R}^{\ell}$, $F: \mathbb{R}^{\ell} \to Y$ such that the following holds to an arbitrarily good approximation:¹

$$f(\{x_1, \dots, x_M\}) = F\left(\sum_{i=1}^M \Phi(x_i)\right)$$

Machine Learning for Point Clouds – Deep Sets

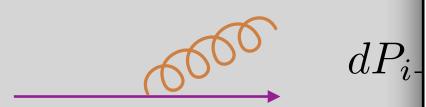
A general permutation-symmetric function is additive in a latent space



General parametrization for a function of sets

Infrared and Collinear (IRC) Safety

QCD has soft and collinear divergences associated with gluon radiation



Infrared (IR) safety - ol

Collinear (C) safety -



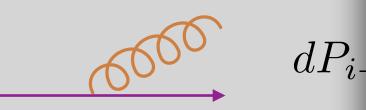
IRC safety is a statement of linearity in energy and continuity in geometry

Theorem: Any IRC-safe observable can be written in the following form:

$$f(\{p_1^{\mu},\ldots,p_M^{\mu}\}) = F\left(\sum_{i=1}^{M} z_i \vec{\Phi}(\hat{p}_i)\right), \quad \hat{p}_i = (y_i,\phi_i).$$

Proof: In 1810.05165.

QCD has soft and collinear divergences associated with gluon radiation



Infrared (IR) safety - ol

Collinear (C) safety –



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IRC safety is a statement of linearity in energy and continuity in geometry

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Proof: In 1810.05165.



ntinuity in metric topology

tinuous at an event \mathcal{E} if, for

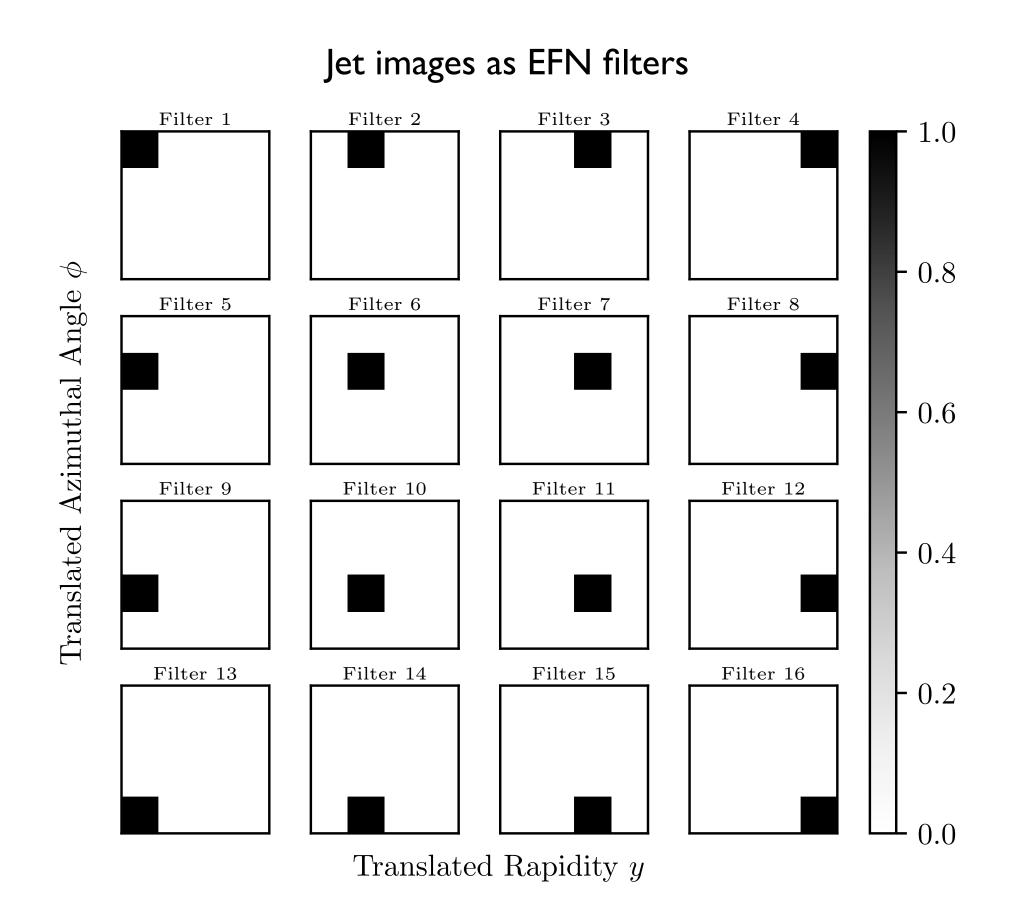
any $\epsilon > 0$, there exists a $\delta > 0$ such that for all events \mathcal{E}' :

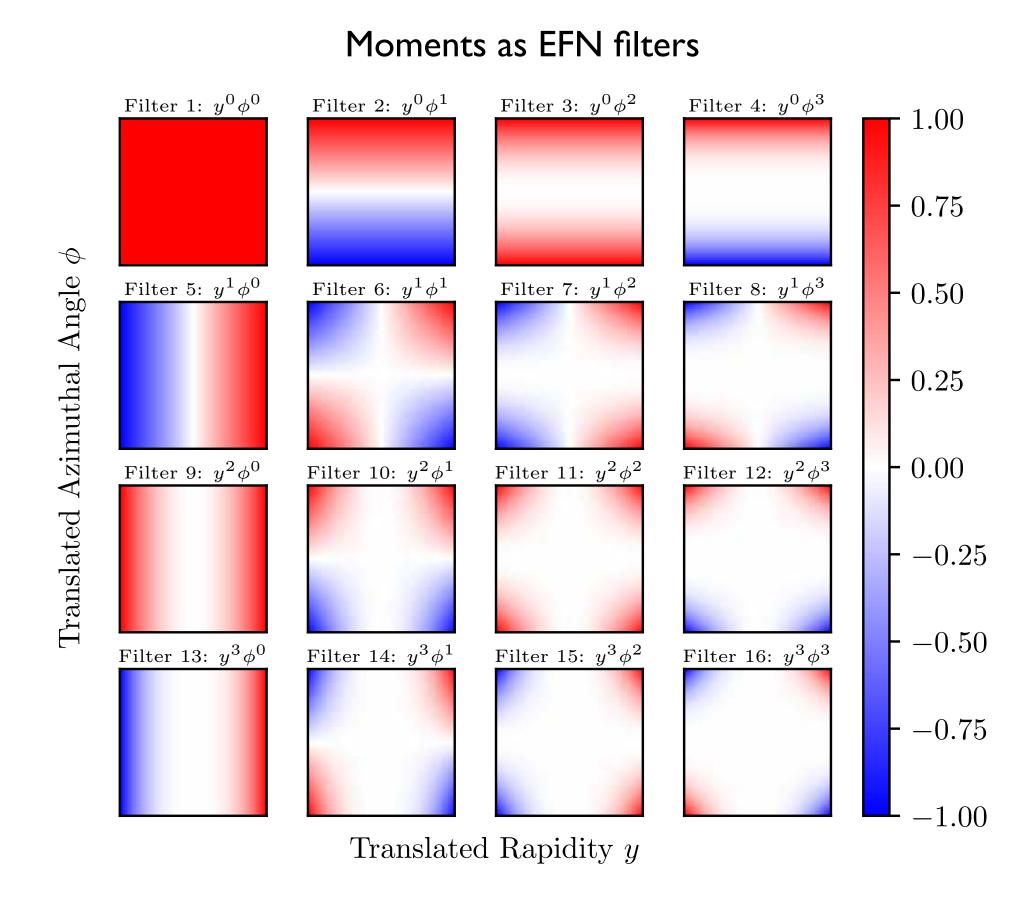
$$\mathrm{EMD}(\mathcal{E}, \mathcal{E}') < \delta \implies |\mathcal{O}(\mathcal{E}) - \mathcal{O}(\mathcal{E}')| < \epsilon.$$

‡a negligible set is one that contains no positive-radius EMD-ball

Energy Flow Network Visualization

Visualize EFN observables as 2D filters in the translated rapidity-azimuth plane

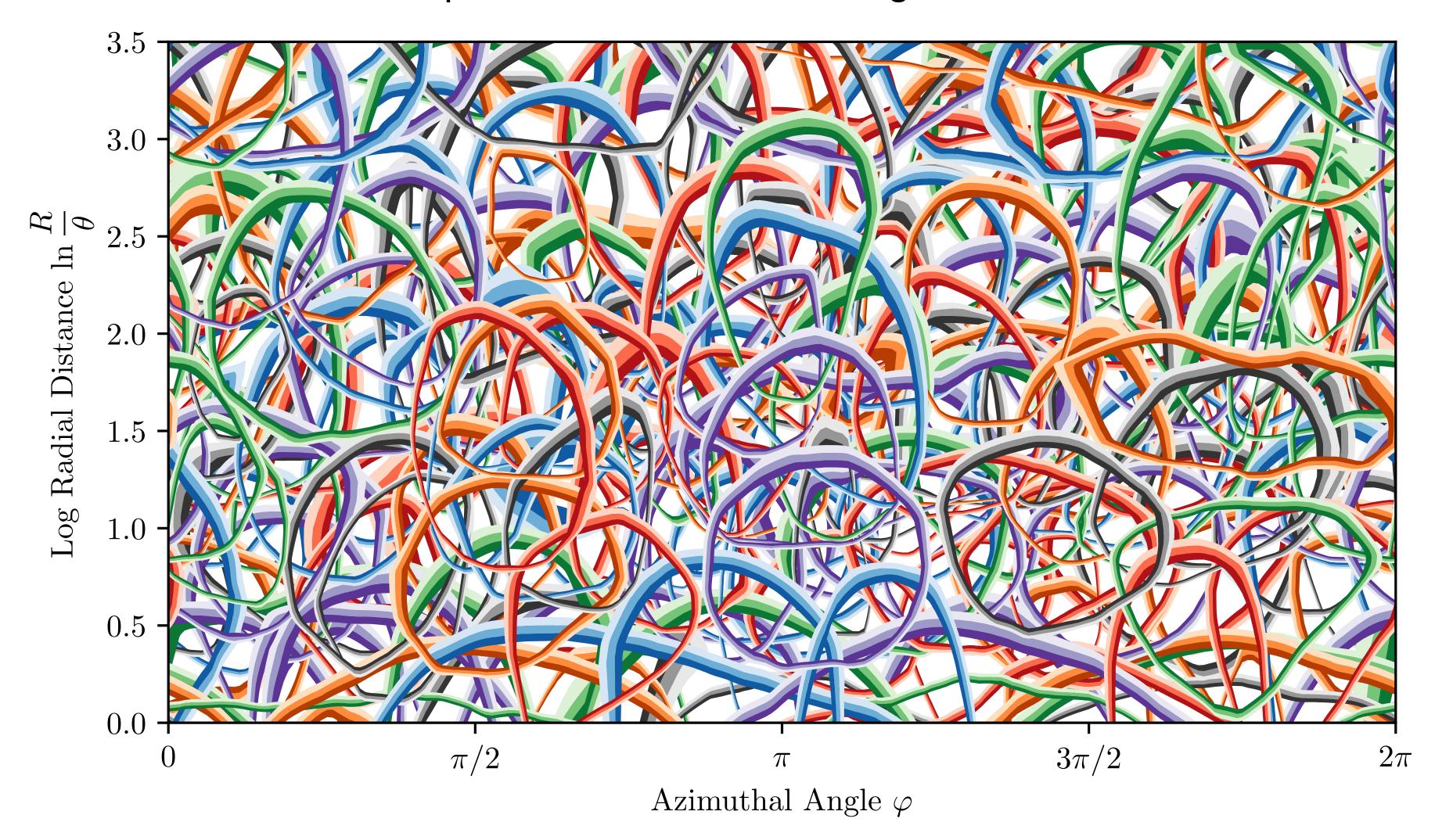




[Donoghue, Low, Pi, <u>PRD 1979</u>; Gur-Ari, Papucci, Perez, <u>1101.2905</u>; **PTK**, Metodiev, Thaler, <u>PRD 2020</u>]

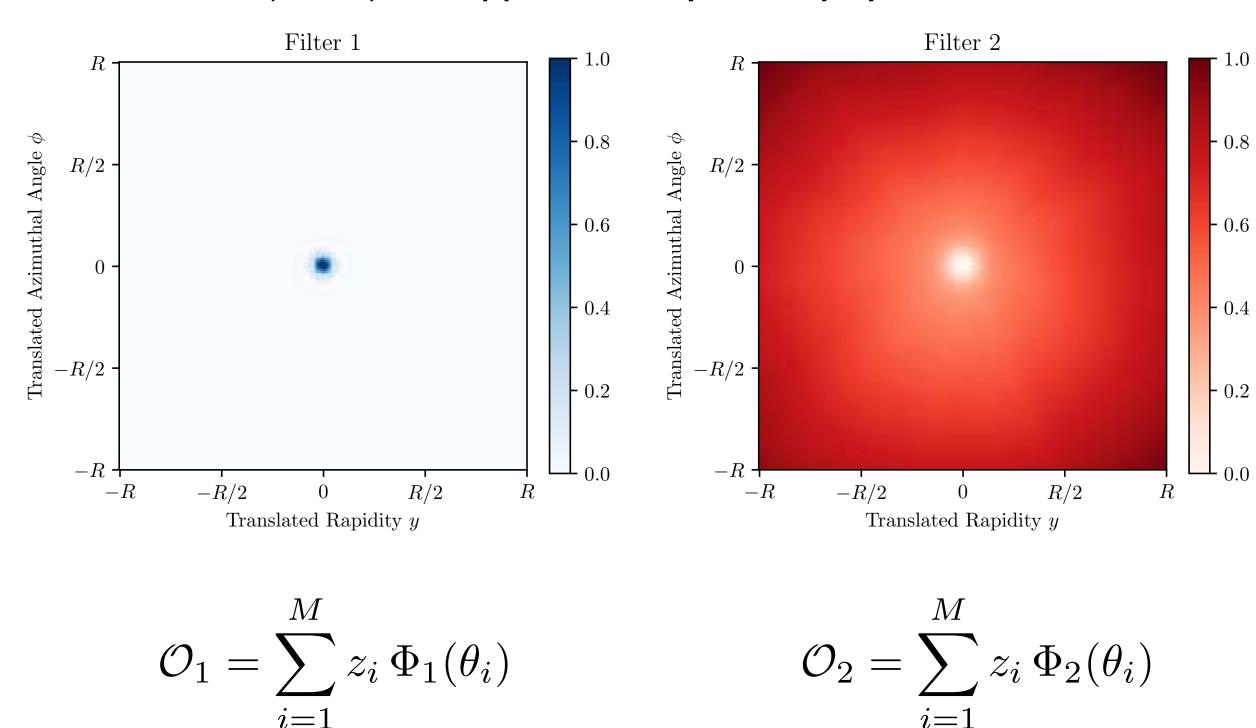
Quark vs. Gluon: Visualizing EFN Filters in the Emission Plane

Transform to polar coordinates and take logarithm of the radius



Quark vs. Gluon: Extracting New Analytic Observables

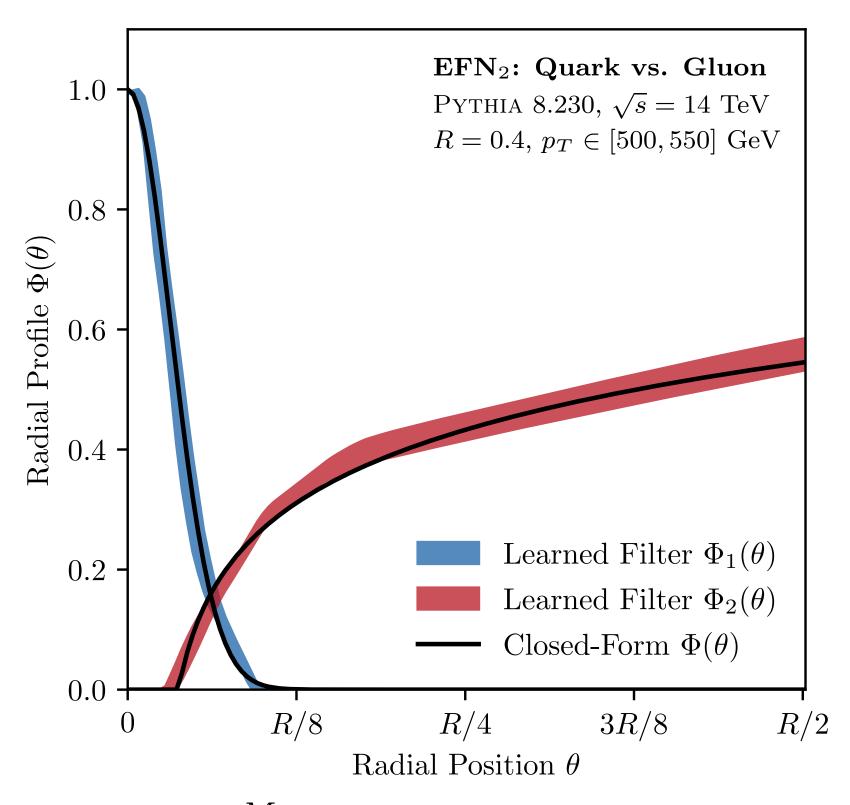
EFN (ℓ = 2) has approximately radially symmetric filters



Separate soft and collinear phase space regions, e.g. collinear drop

[Chien, Stewart, JHEP 2020]

Average of radial slices



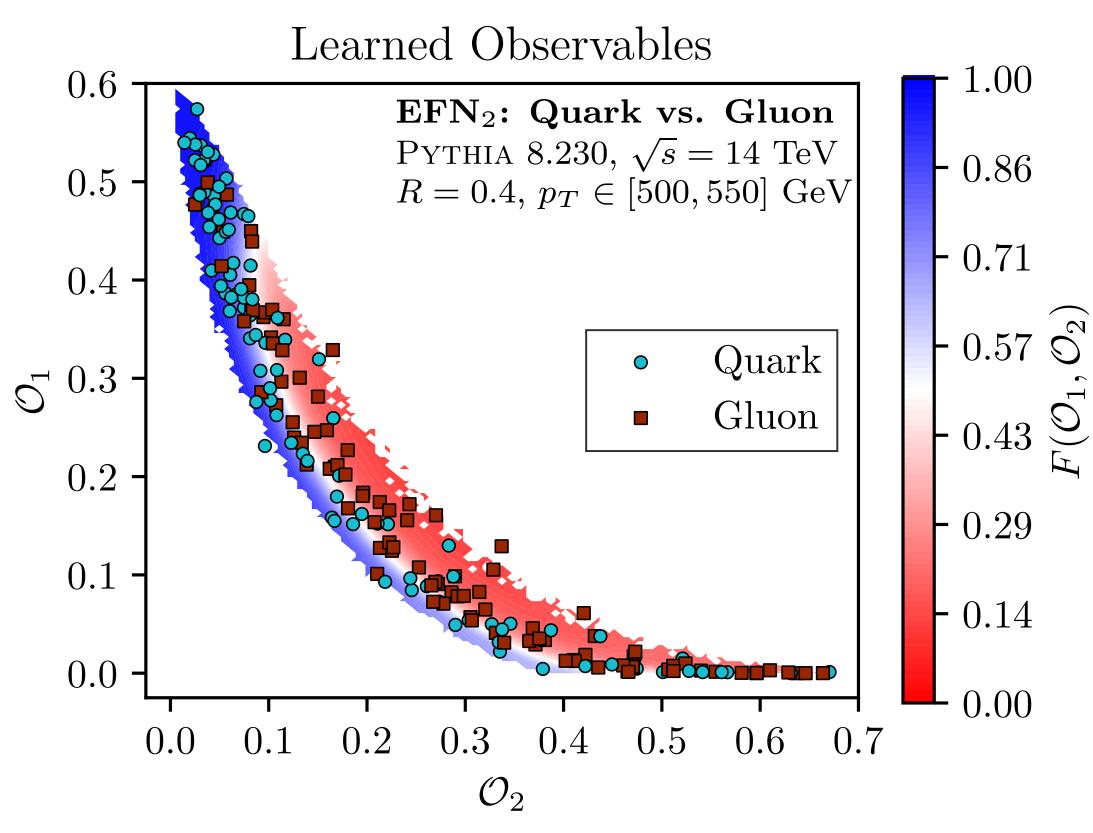
Fit analytic forms:

$$A_{r_0} = \sum_{i=1}^{M} z_i e^{-\theta_i^2/r_0^2},$$

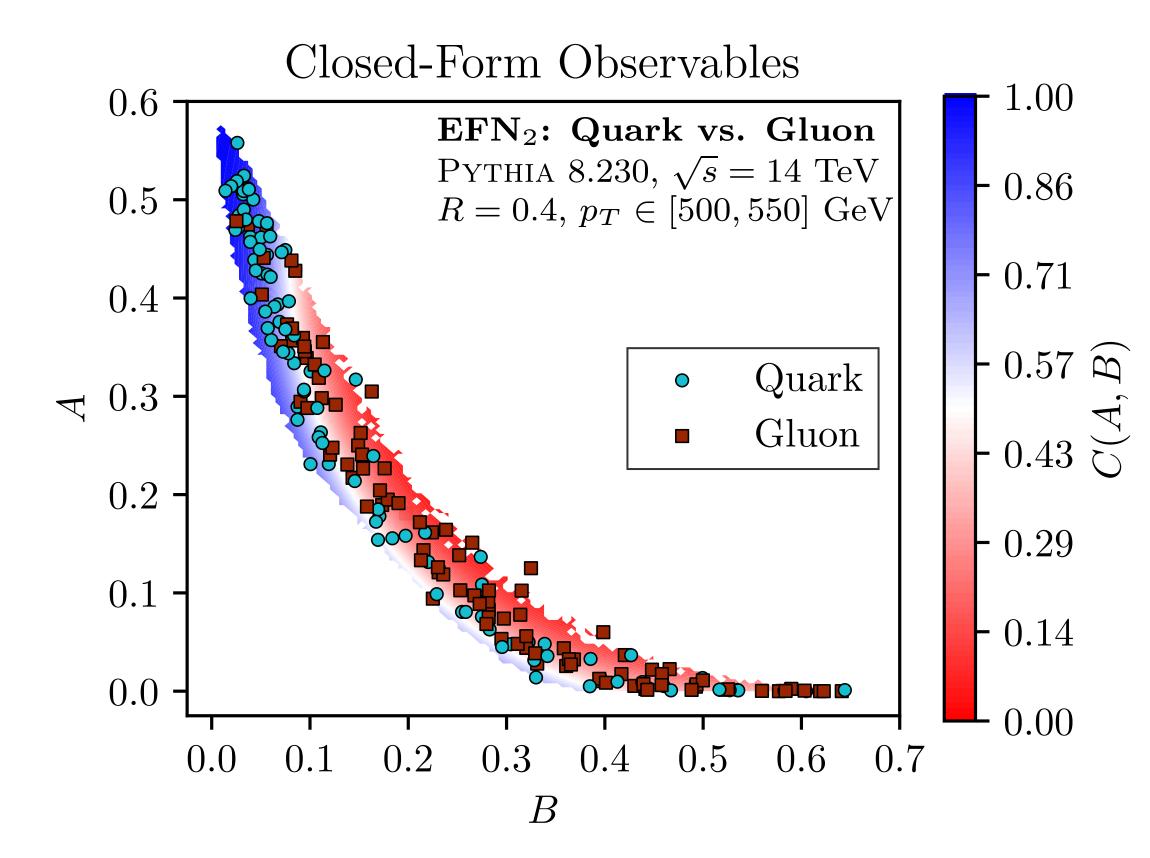
$$B_{r_1,\beta} = \sum_{i=1}^{M} z_i \ln(1 + \beta(\theta_i - r_1))\Theta(\theta_i - r_1)$$

Quark vs. Gluon: Extracting New Analytic Observables

Visualize F in the two dimensional $(\mathcal{O}_1, \mathcal{O}_2)$ phase space



Learned with EFN ($\ell=2$)



Analytic Fit

Squared distance from a point:

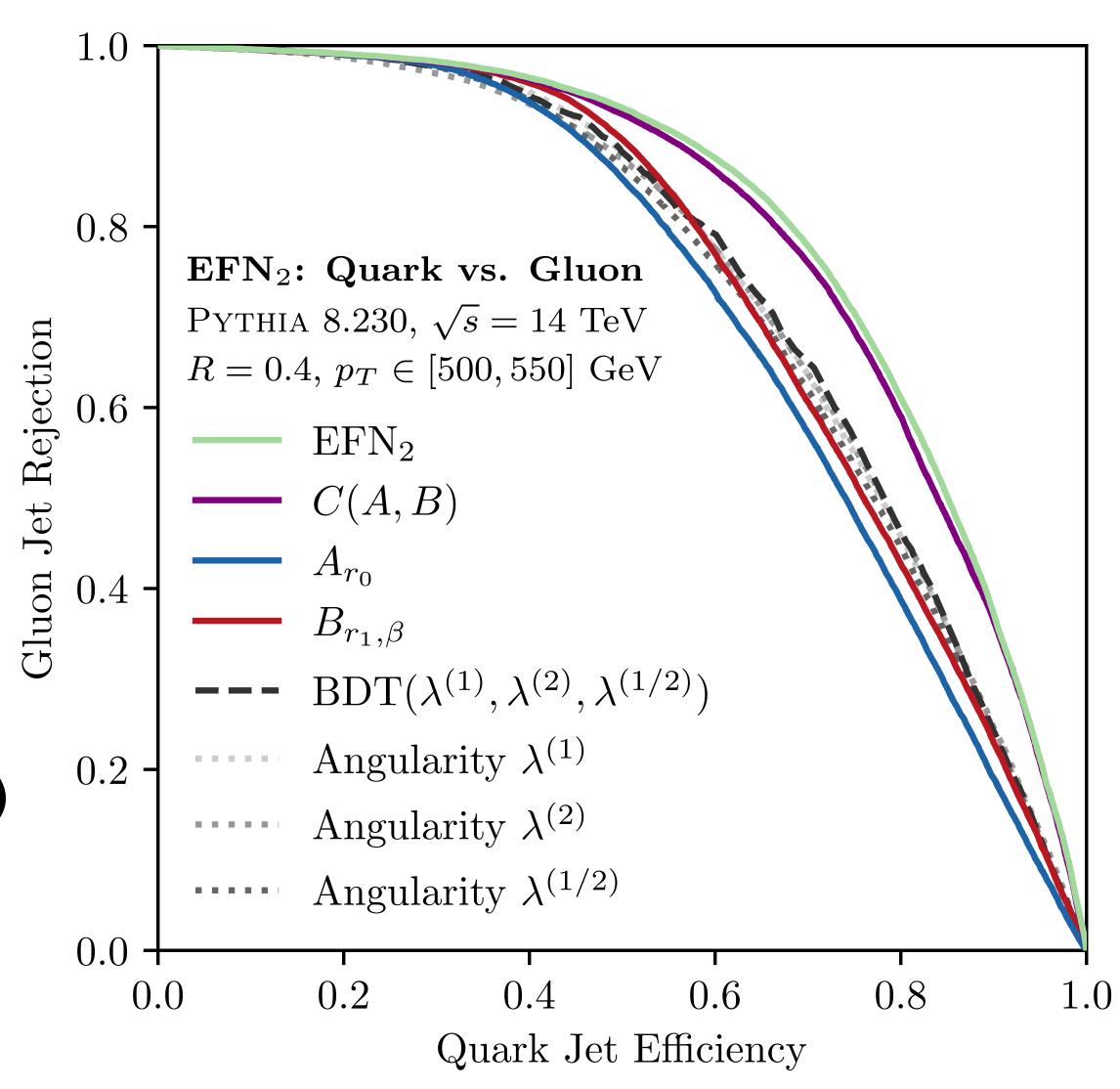
$$C(A,B) = (A - a_0)^2 + (B - b_0)^2$$

Quark vs. Gluon: Benchmarking New Analytic Observables

A, B observables individually comparable to angularities

C(A,B) vastly exceeds multivariate combination (BDT) of angularities

Extracted C(A,B) is comparable to EFN ($\ell=2$)



OmniFold

[Richardson, JOSA 1972; Lucy, AJ 1974; D'Agostini, NIMPA 1995]

Maximum likelihood, histogram-based unfolding method for a small number of observables

Choose observable(s) and binning at detector-level and particle-level

measured distribution: $m_i = \Pr(\text{measure } i)$ true distribution: $t_j^{(0)} = \Pr(\text{truth is } j)$

Calculate response matrix R_{ij} from generated/simulated pairs of events

$$R_{ij} = \Pr(\text{measure } i \mid \text{truth is } j)$$

Calculate new particle-level distribution using Bayes' theorem

$$t_{j}^{(n)} = \sum_{i} \Pr(\text{truth}_{n-1} \text{ is } j \mid \text{measure } i) \times \Pr(\text{measure } i)$$

$$= \sum_{i} \frac{R_{ij}t_{j}^{(n-1)}}{\sum_{k} R_{ik}t_{k}^{(n-1)}} \times m_{i}$$

Iterate procedure to remove dependence on prior

Consider a situation with two particle-level bins and two detector-level bins

$$t_j^{(0)} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_j$$

$$m_i = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

$$R_{ij} = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \end{pmatrix}_{ij}$$

Uniform prior

Bins are measured equally

Bin I reconstructed perfectly Bin 2 reconstructed equally

[Richardson, JOSA 1972; Lucy, AJ 1974; D'Agostini, NIMPA 1995]

Maximum likelihood, histogram-based unfolding method for a small number of observables

Choose observable(s) and binning at detector-level and particle-level

measured distribution: $m_i = \Pr(\text{measure } i)$ true distribution: $t_i^{(0)} = \Pr(\text{truth is } j)$

Calculate response matrix R_{ii} from generated/simulated pairs of events

$$R_{ij} = \Pr(\text{measure } i \mid \text{truth is } j)$$

Calculate new particle-level distribution using Bayes' theorem

$$t_{j}^{(n)} = \sum_{i} \Pr(\text{truth}_{n-1} \text{ is } j \mid \text{measure } i) \times \Pr(\text{measure } i)$$

$$= \sum_{i} \frac{R_{ij}t_{j}^{(n-1)}}{\sum_{k} R_{ik}t_{k}^{(n-1)}} \times m_{i}$$

Iterate procedure to remove dependence on prior

Consider a situation with two particle-level bins and two detector-level bins

$$t_j^{(0)} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_j \qquad m_i = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_i$$

$$m_i = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_i$$

$$R_{ij} = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \end{pmatrix}_{ii}$$

Uniform prior

Bins are measured equally

Bin I reconstructed perfectly Bin 2 reconstructed equally

$$t_{j}^{(1)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i}$$

After one iteration

Maximum likelihood, histogram-based unfolding method for a small number of observables

Choose observable(s) and binning at detector-level and particle-level

measured distribution: $m_i = \Pr(\text{measure } i)$ true distribution: $t_j^{(0)} = \Pr(\text{truth is } j)$

Calculate response matrix R_{ii} from generated/simulated pairs of events

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$$= \sum_{i} \frac{R_{ij}t_{j}^{(n-1)}}{\sum_{k} R_{ik}t_{k}^{(n-1)}} \times m_{i}$$

Iterate procedure to remove dependence on prior

Consider a situation with two particle-level bins and two detector-level bins

$$f_j^{(0)} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_j$$

$$m_i = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_i$$

$$R_{ij} = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \end{pmatrix}_{i}$$

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$$t_{j}^{(1)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} = \begin{pmatrix} \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{2} + 0}{\frac{1}{3}} \\ \frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4} \\ \frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \\ \frac{2}{3} \end{pmatrix}_{j}$$
After one iteration

Maximum likelihood, histogram-based unfolding method for a small number of observables

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Calculate new particle-level distribution using Bayes' theorem

$$t_{j}^{(n)} = \sum_{i} \Pr(\text{truth}_{n-1} \text{ is } j \mid \text{measure } i) \times \Pr(\text{measure } i)$$

$$= \sum_{i} \frac{R_{ij}t_{j}^{(n-1)}}{\sum_{k} R_{ik}t_{k}^{(n-1)}} \times m_{i}$$

Iterate procedure to remove dependence on prior

Consider a situation with two particle-level bins and two detector-level bins

$$m_{i} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{j} \qquad m_{i} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} \qquad R_{ij} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

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$$t_{j}^{(1)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} = \begin{pmatrix} \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{2} + 0}{\frac{1}{3}} \\ \frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4} \\ \frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \\ \frac{2}{3} \end{pmatrix}_{j}$$
After one iteration

•

Correct truth distribution obtained as
$$n \to \infty$$

$$t_{j}^{(n)} = \sum_{i} \frac{\left(\frac{1}{n+1} \frac{n}{2(n+1)}\right)_{ij}}{\left(\frac{n+2}{2(n+1)} \frac{n}{2(n+1)}\right)_{i}} \times \left(\frac{\frac{1}{2}}{\frac{1}{2}}\right)_{i} = \left(\frac{1}{n+2}\right)_{i} \to \left(0\right)_{1}$$

Consider a situation with two particle-level bins and two detector-level bins

$$t_j^{(0)} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_i$$

$$m_i = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

$$R_{ij} = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \end{pmatrix}_{ij}$$

Uniform prior

Bins are measured equally

Bin I reconstructed perfectly Bin 2 reconstructed equally

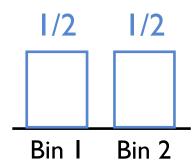
$$t_{j}^{(1)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} = \begin{pmatrix} \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{2} + 0}{\frac{1}{3}} \\ \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4}}{\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}_{j}$$
After one iteration

•

$$t_{j}^{(n)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{n+1} & \frac{n}{2(n+1)} \\ 0 & \frac{n}{2(n+1)} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{n+2}{2(n+1)} & \frac{n}{2(n+1)} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} = \begin{pmatrix} \frac{1}{n+2} \\ \frac{n+1}{n+2} \\ \frac{n}{n+2} \end{pmatrix}_{i} \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{j}$$

[Richardson, JOSA 1972; Lucy, AJ 1974; D'Agostini, NIMPA 1995]

prior



Consider a situation with two particle-level bins and two detector-level bins

$$m_i = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_i$$

$$m_i = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_i$$

Uniform prior

Bins are measured equally

Bin I reconstructed perfectly Bin 2 reconstructed equally

$$t_{j}^{(1)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} = \begin{pmatrix} \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{2} + 0}{\frac{1}{3}} \\ \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4}}{\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}_{j}$$
After one iteration

Correct truth distribution obtained as $n \to \infty$

IBU as Reweighting

[Richardson, JOSA 1972; Lucy, AJ 1974; D'Agostini, NIMPA 1995]

response I prior 1/2 detector Bin I Bin 2 Bin 2 Bin I

Consider a situation with two particle-level bins and two detector-level bins

$$m_{i} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i}$$
 $m_{i} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}_{i}$
 $R_{ij} = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i}$

Uniform prior

Bins are measured equally

Bin I reconstructed perfectly Bin 2 reconstructed equally

$$t_{j}^{(1)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} = \begin{pmatrix} \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{2} + 0}{\frac{1}{3}} \\ \frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4} \\ \frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}_{j}$$
After one iteration

After one iteration

$$t_{j}^{(n)} = \sum_{i} \frac{\left(\frac{1}{n+1} \frac{n}{2(n+1)}\right)_{ij}}{\left(\frac{n+2}{2(n+1)} \frac{n}{2(n+1)}\right)_{i}} \times \left(\frac{\frac{1}{2}}{\frac{1}{2}}\right)_{i} = \left(\frac{1}{n+2}\right)_{i} \rightarrow \left(0\right)_{1}$$
Correct truth distribution obtained as $n \to \infty$

IBU as Reweighting

[Richardson, JOSA 1972; Lucy, AJ 1974; D'Agostini, NIMPA 1995]

but I actually detected ...

Consider a situation with two particle-level bins and two detector-level bins

$$m_{i} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} \qquad R_{ij} = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \\ 0 & \frac{1}{2} \end{pmatrix}_{ij}$$

Uniform prior

Bins are measured equally

Bin I reconstructed perfectly Bin 2 reconstructed equally

$$t_{j}^{(1)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} = \begin{pmatrix} \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{2} + 0}{\frac{1}{3}} \\ \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4}}{\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}_{j}$$
After one iteration

•

Correct truth distribution obtained as
$$n \to \infty$$

$$\frac{\left(\frac{1}{n+1} \frac{n}{2(n+1)}\right)}{\left(\frac{n+2}{2(n+1)} \frac{n}{2(n+1)}\right)_i} \times \left(\frac{\frac{1}{2}}{\frac{1}{2}}\right)_i = \left(\frac{1}{n+2}\right)_j \to \left(0\right)_1$$

IBU as Reweighting

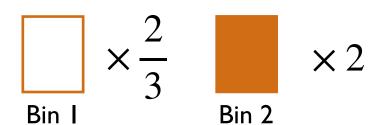
[Richardson, JOSA 1972; Lucy, AJ 1974; D'Agostini, NIMPA 1995]

response I prior 1/2 1/2 detector Bin I Bin 2

reweight bins to match

Bin 2

Bin I



but I actually detected ...

Consider a situation with two particle-level bins and two detector-level bins

$$m_{i} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i}$$
 $m_{i} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}_{ij}$
 $R_{ij} = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \\ 0 \end{pmatrix}_{ij}$

Uniform prior

Bins are measured equally

Bin I reconstructed perfectly Bin 2 reconstructed equally

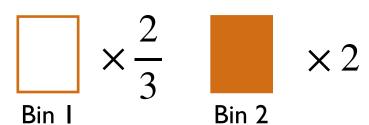
$$t_{j}^{(1)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} = \begin{pmatrix} \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{2} + 0}{\frac{1}{3}} \\ \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4}}{\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}_{j}$$
After one iteration

Correct truth distribution obtained as $n \to \infty$

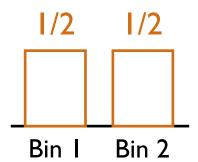
IBU as Reweighting

[Richardson, JOSA 1972; Lucy, AJ 1974; D'Agostini, NIMPA 1995]

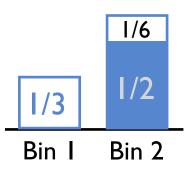
reweight bins to match



but I actually detected ...



pull reweighting back to truth level



Consider a situation with two particle-level bins and two detector-level bins

$$m_{i} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i}$$
 $m_{i} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}_{i}$
 $R_{ij} = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \\ i \end{pmatrix}_{i}$

Uniform prior

Bins are measured equally

Bin I reconstructed perfectly Bin 2 reconstructed equally

Correct truth distribution

$$t_{j}^{(1)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} = \begin{pmatrix} \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{2} + 0}{\frac{1}{3}} \\ \frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4} \\ \frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}_{j}$$
After one iteration

•

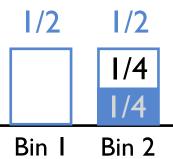
 $\frac{\binom{1}{n+1} \frac{n}{2(n+1)}}{0 \frac{n}{2(n+1)} \frac{n}{2(n+1)}} \times \binom{\frac{1}{2}}{\frac{1}{2}} = \binom{\frac{1}{n+2}}{\frac{n+1}{n+2}} \to \binom{0}{1}_{j}$ obtained as $n \to \infty$

At the nth iteration

IBU as Reweighting

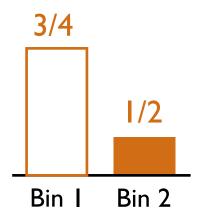
[Richardson, JOSA 1972; Lucy, AJ 1974; D'Agostini, NIMPA 1995]

prior

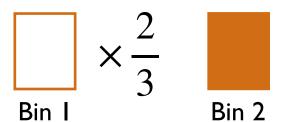




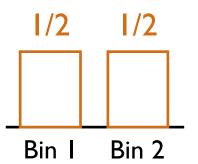




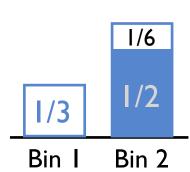
reweight bins to match



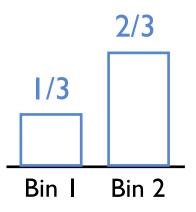
but I actually detected ...



pull reweighting back to truth level



new estimate of truth



Consider a situation with two particle-level bins and two detector-level bins

$$t_j^{(0)} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_j$$

$$m_i = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_i$$

$$R_{ij} = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \end{pmatrix}_{ij}$$

Uniform prior

Bins are measured equally

Bin I reconstructed perfectly Bin 2 reconstructed equally

$$t_{j}^{(1)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} = \begin{pmatrix} \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{2} + 0}{\frac{1}{3}} \\ \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4}}{\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}_{j}$$
After one iteration

•

$${\binom{n}}{n+1} = \sum_{i=1}^{n} \frac{\left(\frac{1}{n+1} + \frac{n}{2(n+1)}\right)_{ij}}{\left(\frac{n+2}{2(n+1)} + \frac{n}{2(n+1)}\right)} \times {\binom{1}{2}} = {\binom{1}{n+2} \choose \frac{n+1}{2(n+1)}}$$

Correct truth distribution obtained as $n \to \infty$

$$\frac{\left(\frac{n+2}{2(n+1)} \quad \frac{n}{2(n+1)}\right)_{i}}{\left(\frac{n+2}{2(n+1)}\right)_{i}} \quad \left(\frac{1}{2}\right)_{i} \quad \left(\frac{n+1}{n+2}\right)_{j} \quad \left(\frac{n+1}{n+2}\right)_{j}$$

At the nth iteration

IBU as Reweighting

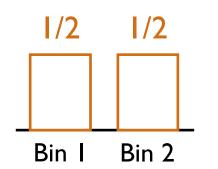
[Richardson, JOSA 1972; Lucy, AJ 1974; D'Agostini, NIMPA 1995]

reweight bins to match

 $\frac{2}{3}$ Bin I

Bin 2

but I actually detected ...



pull reweighting back to truth level

new estimate of truth



Consider a situation with two particle-level bins and two detector-level bins

$$m_{i} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i}$$
 $m_{i} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}_{ij}$
 $R_{ij} = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \\ 0 \end{pmatrix}_{ij}$

Uniform prior

Bins are measured equally

Bin I reconstructed perfectly Bin 2 reconstructed equally

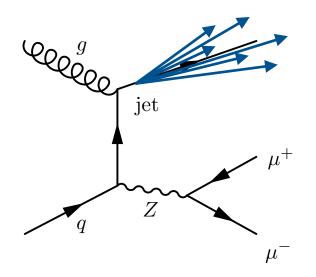
$$t_{j}^{(1)} = \sum_{i} \frac{\begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} \end{pmatrix}_{ij}}{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}_{i}} \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}_{i} = \begin{pmatrix} \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{2} + 0}{\frac{1}{3}} \\ \frac{\frac{1}{2} \times \frac{4}{3} \times \frac{1}{4} + \frac{1}{2} \times 4 \times \frac{1}{4}}{\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}_{j}$$
After one iteration

Correct truth distribution obtained as $n \to \infty$

$$t_{j}^{(n)} = \sum_{i} \frac{\left(\frac{n+1}{2(n+1)}\right)_{ij}}{\left(\frac{n+2}{2(n+1)}\right)_{i}} \times \left(\frac{\frac{1}{2}}{\frac{1}{2}}\right)_{i} = \left(\frac{\frac{1}{n+2}}{\frac{n+1}{n+2}}\right)_{j} \to \left(0\right)_{j}$$

At the nth iteration

OmniFold Results by Event Representation



User is free to choose event representation in the OmniFold procedure

OMNIFOLD – full phase space information



MULTIFOLD – multiple observables



UNIFOLD – single observable, essentially unbinned IBU

	Observable						
Method	m	M	w	$\ln ho$	$ au_{21}$	z_g	
OmniFold	2.77	0.33	0.10	0.35	0.53	0.68	
MultiFold	3.80	0.89	0.09	0.37	0.26	0.15	
UniFold	8.82	1.46	0.15	0.59	1.11	0.59	
IBU	9.31	1.51	0.11	0.71	1.10	0.37	
Data	24.6	130	15.7	14.2	11.1	3.76	
Generation	3.62	15	22.4	19	20.8	3.84	
	mass	mult.	width	<u> </u>	<u> </u>	N-su	i ubj. r
	groomed mass						

Evaluate performance using triangular discriminator

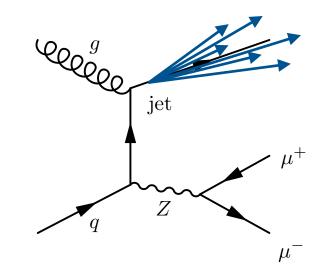
$$\Delta(p,q) = \frac{1}{2} \int d\lambda \, \frac{(p(\lambda) - q(\lambda))^2}{p(\lambda) + q(\lambda)} (\times 10^3)$$

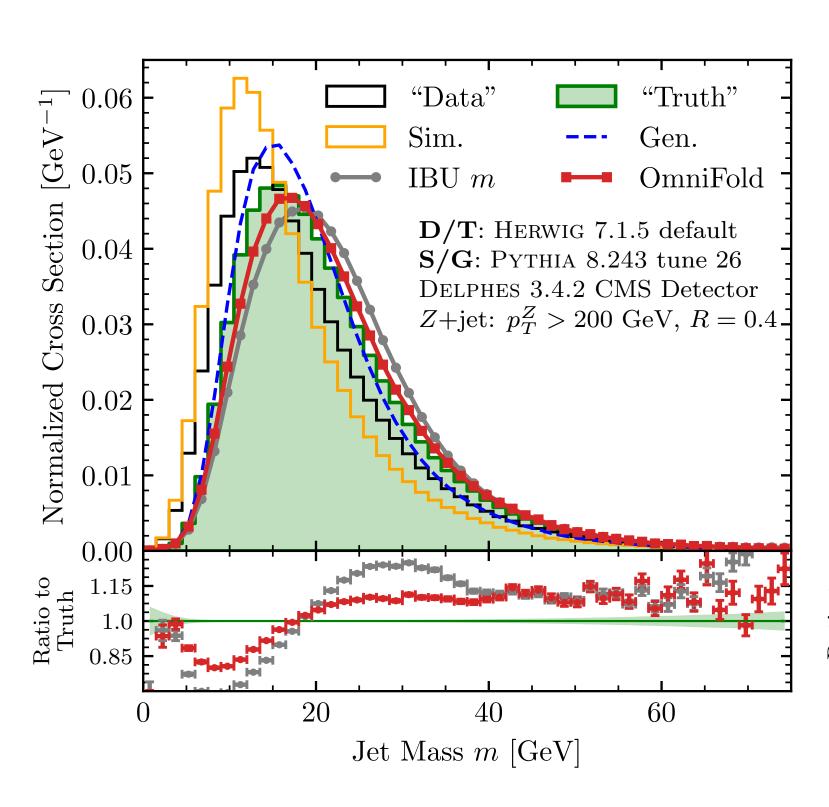
OMNIFOLD/MULTIFOLD outperforms IBU on all observables!

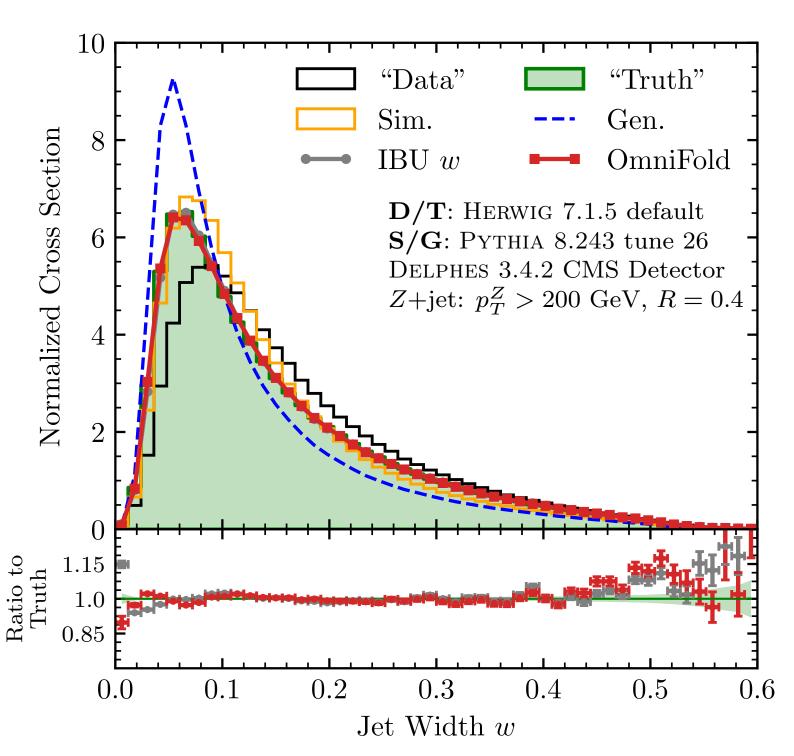
Single MULTIFOLD training based on all six observables

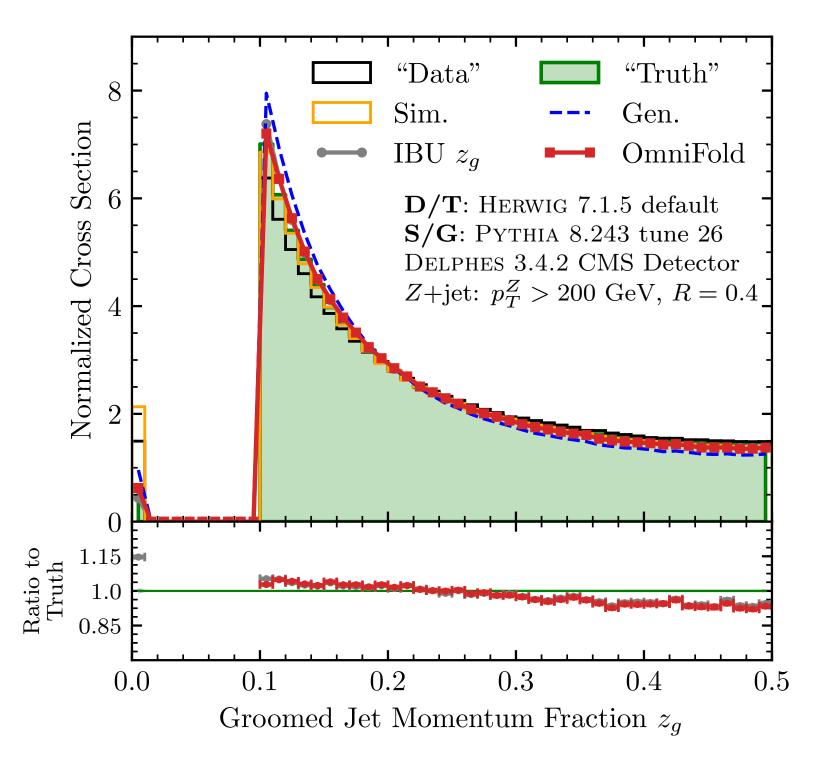
UNIFOLD is similar to or outperforms IBU

Additional OmniFolded Distributions









Jet mass affected by particle masses

$$m_J^2 = \left(\sum_{i \in \mathbf{jet}} p_i^{\mu}\right)^2$$

IRC-safe observables easier to unfold

$$w = \frac{1}{\sum_{i} p_{Tj}} \sum_{i} p_{Ti} \sqrt{(y_i - y_J)^2 + (\phi_i - \phi_J)^2}$$

 z_g remarkably stable under choice of method

 $z_g = p_T$ fraction of first splitting to pass soft drop

OmniFold Etymology

The Mountain sat upon the Plain In his tremendous Chair — His observation **omnifold**, His inquest, everywhere —

The Seasons played around his knees Like Children round a sire – Grandfather of the Days is He Of Dawn, the Ancestor –

Emily Dickinson, #975

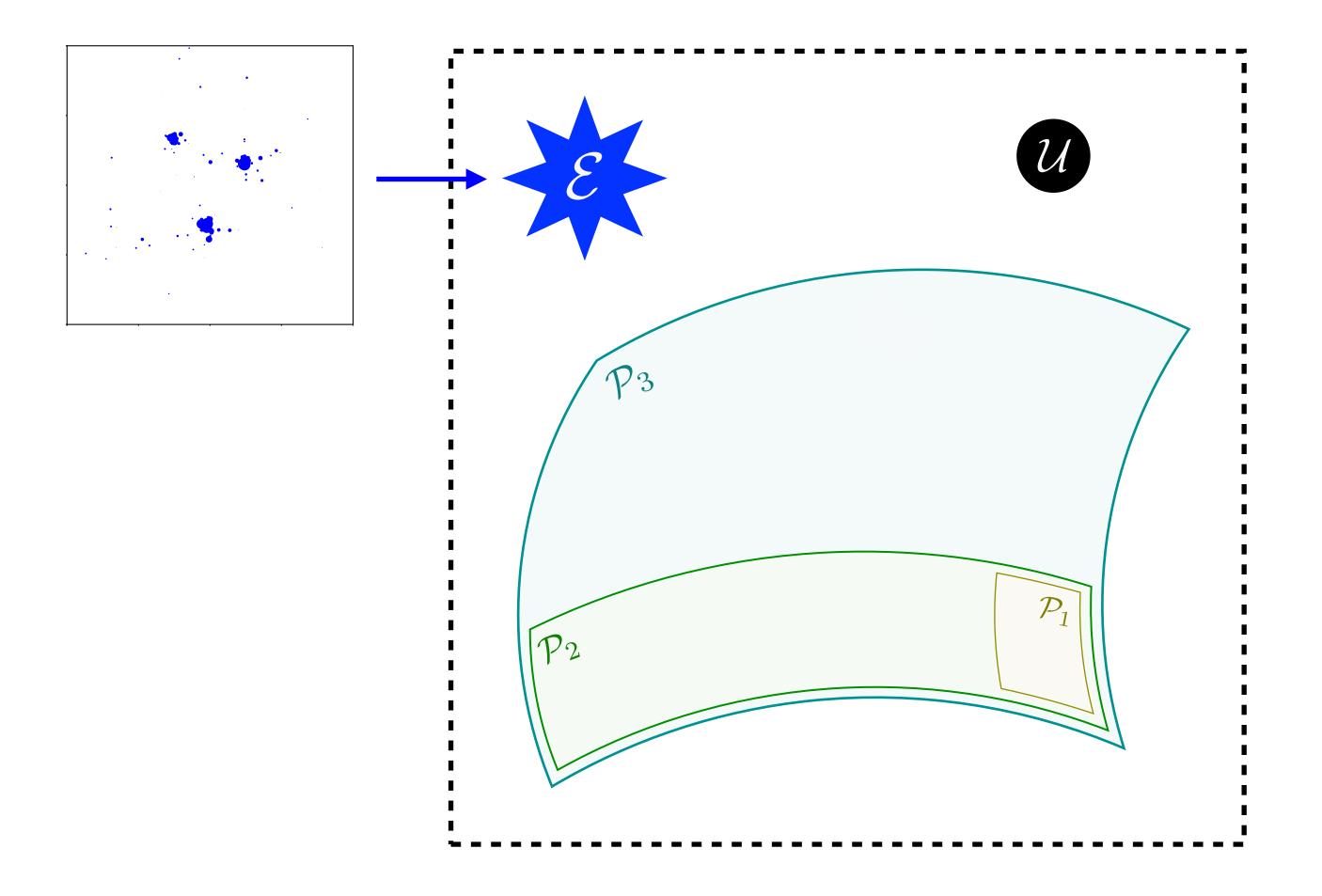


Energy Mover's Distance

N-particle Manifolds in the Space of Events

[PTK, Metodiev, Thaler, JHEP 2020]

$$\mathcal{P}_N$$
 = set of all N-particle configurations = $\left\{\sum_{i=1}^N E_i \, \delta(\hat{n} - \hat{n}_i) \,\middle|\, E_i \geq 0\right\}$



•

$$\mathcal{P}_N \supset \mathcal{P}_{N-1} \supset \cdots \supset \mathcal{P}_3 \supset \mathcal{P}_2 \supset \mathcal{P}_1$$

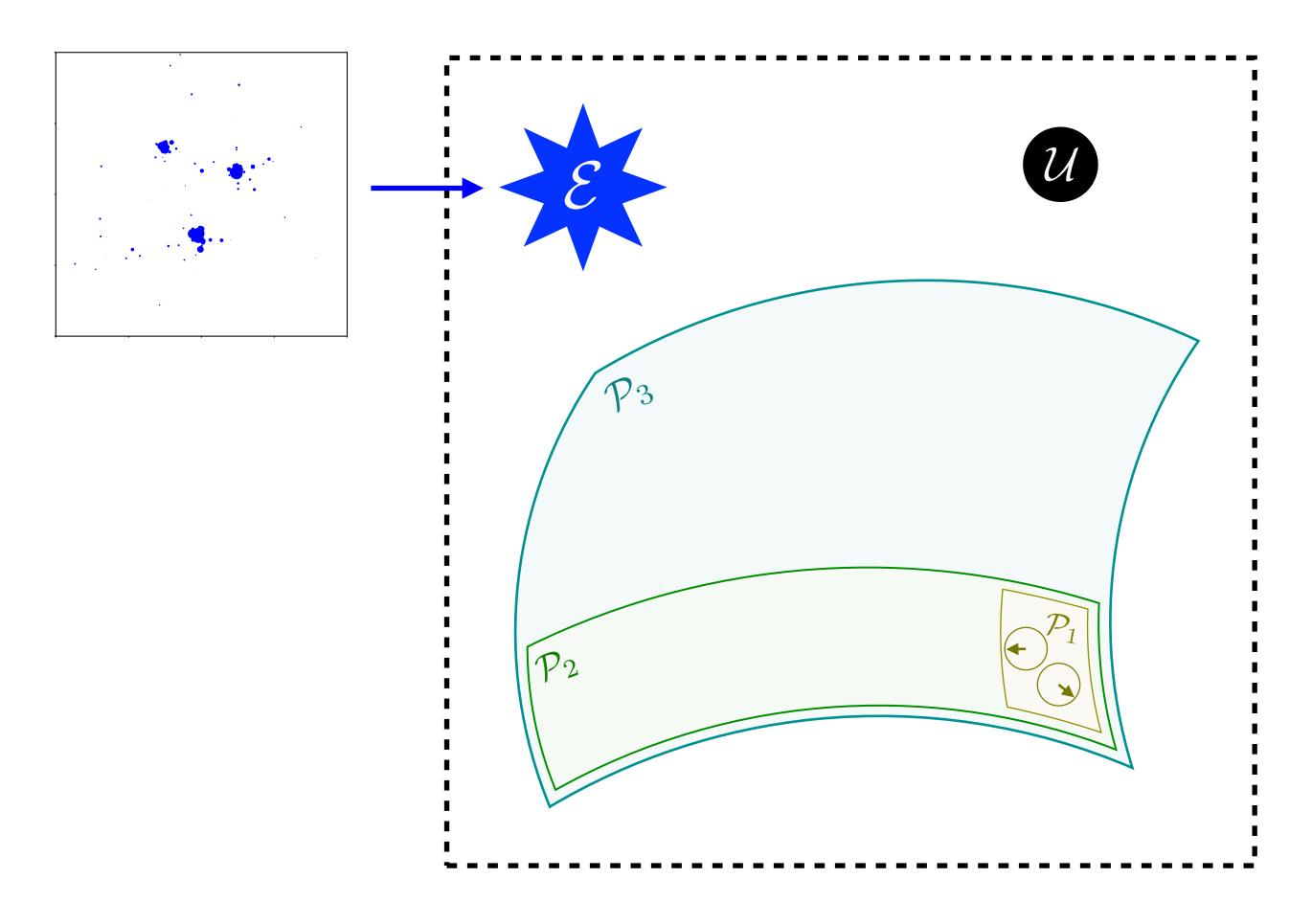
by soft and collinear limits

Uniform event, not contained in any P_N

N-particle Manifolds in the Space of Events

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 \mathcal{P}_1 : manifold of events with one particle

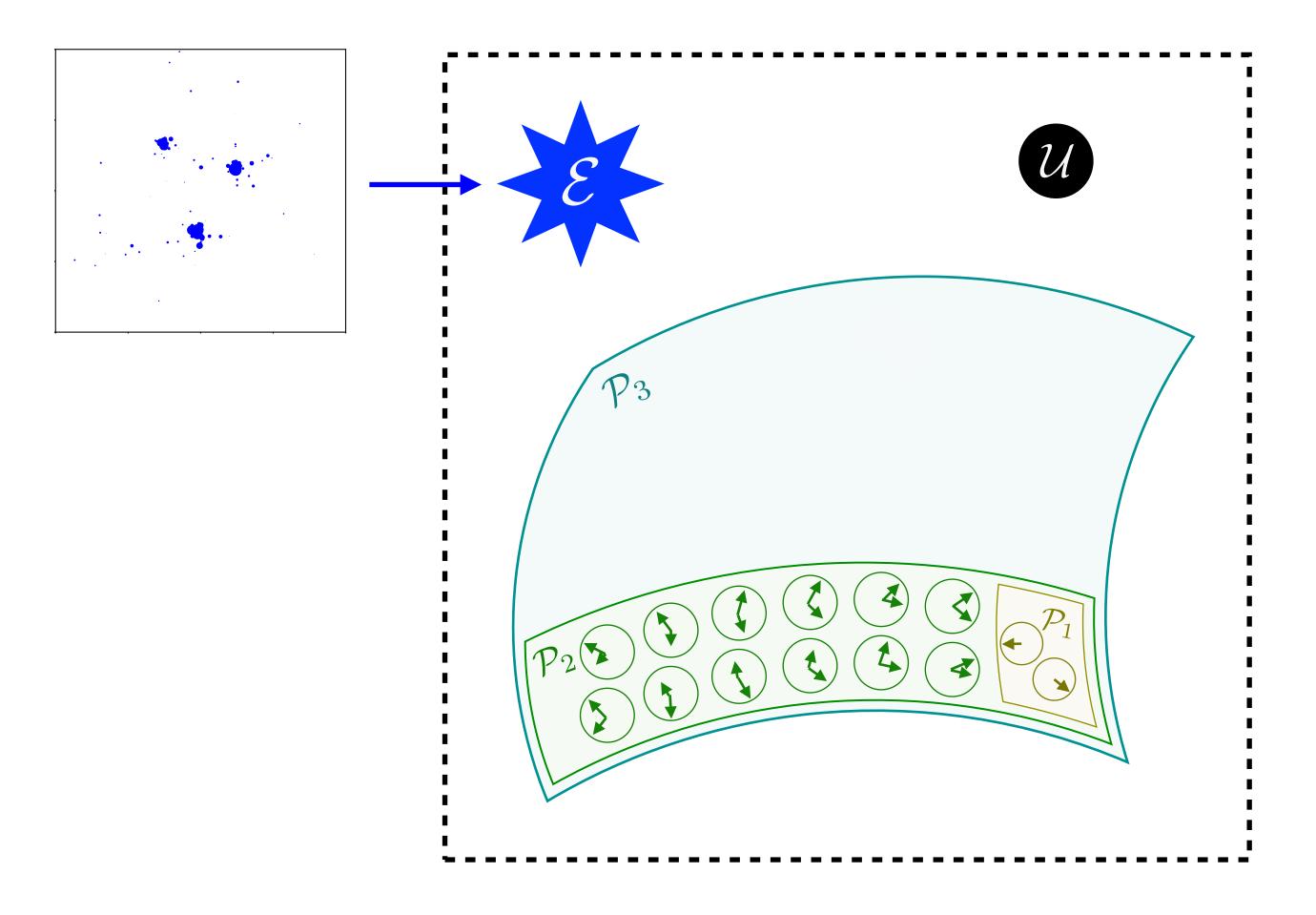
•

$$\mathcal{P}_N \supset \mathcal{P}_{N-1} \supset \cdots \supset \mathcal{P}_3 \supset \mathcal{P}_2 \supset \mathcal{P}_1$$

by soft and collinear limits

Uniform event, not contained in any P_N

$$\mathcal{P}_N$$
 = set of all N-particle configurations = $\left\{\sum_{i=1}^N E_i \, \delta(\hat{n} - \hat{n}_i) \, \middle| \, E_i \geq 0 \right\}$



 \mathcal{P}_1 : manifold of events with one particle

 \mathcal{P}_2 : manifold of events with two particles

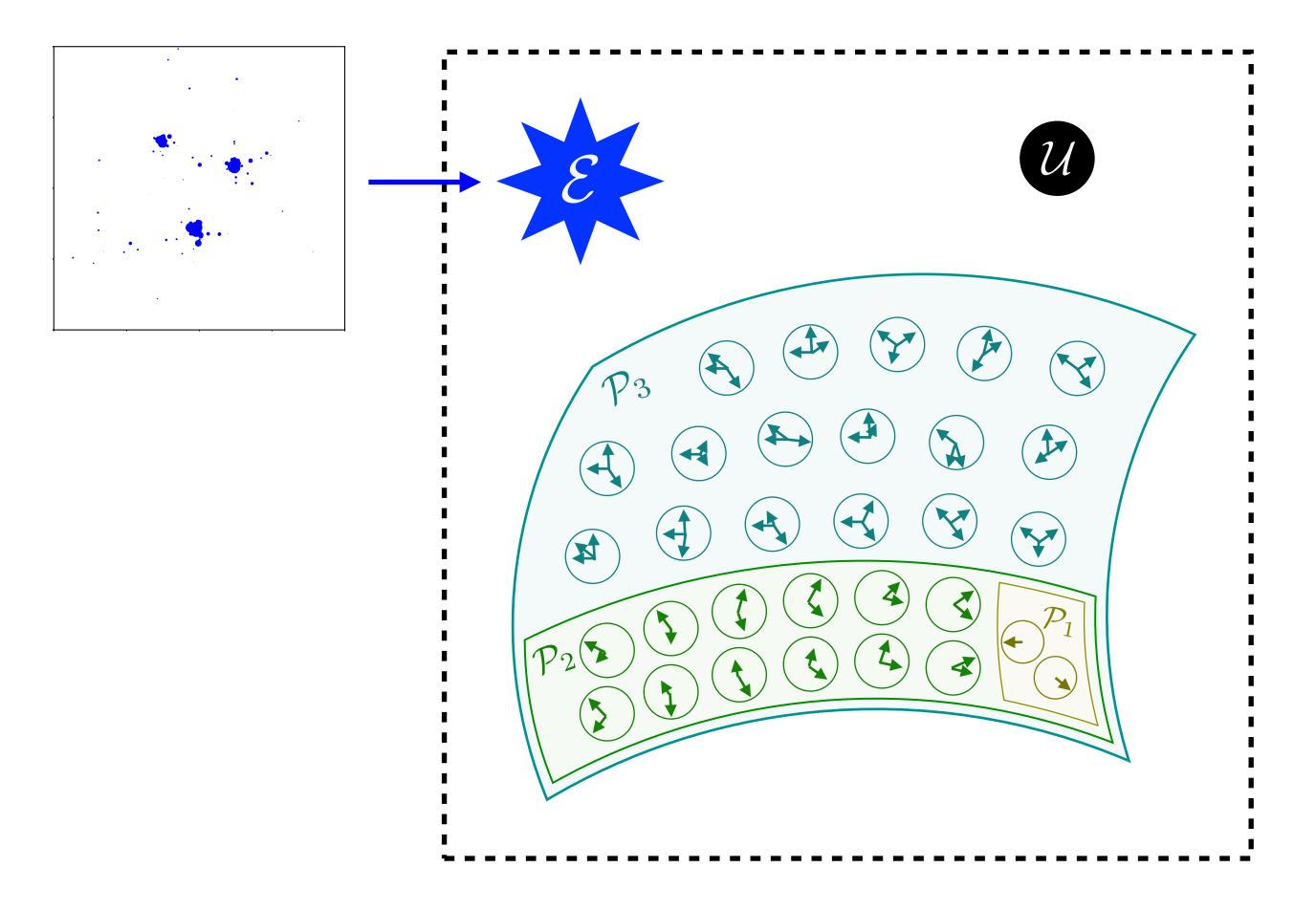
•

$$\mathcal{P}_N \supset \mathcal{P}_{N-1} \supset \cdots \supset \mathcal{P}_3 \supset \mathcal{P}_2 \supset \mathcal{P}_1$$

by soft and collinear limits

Uniform event, not contained in any P_N

$$\mathcal{P}_N$$
 = set of all N-particle configurations = $\left\{\sum_{i=1}^N E_i \, \delta(\hat{n} - \hat{n}_i) \mid E_i \geq 0\right\}$



 \mathcal{P}_1 : manifold of events with one particle

 \mathcal{P}_2 : manifold of events with two particles

 \mathcal{P}_3 : manifold of events with three particles

•

$$\mathcal{P}_N \supset \mathcal{P}_{N-1} \supset \cdots \supset \mathcal{P}_3 \supset \mathcal{P}_2 \supset \mathcal{P}_1$$

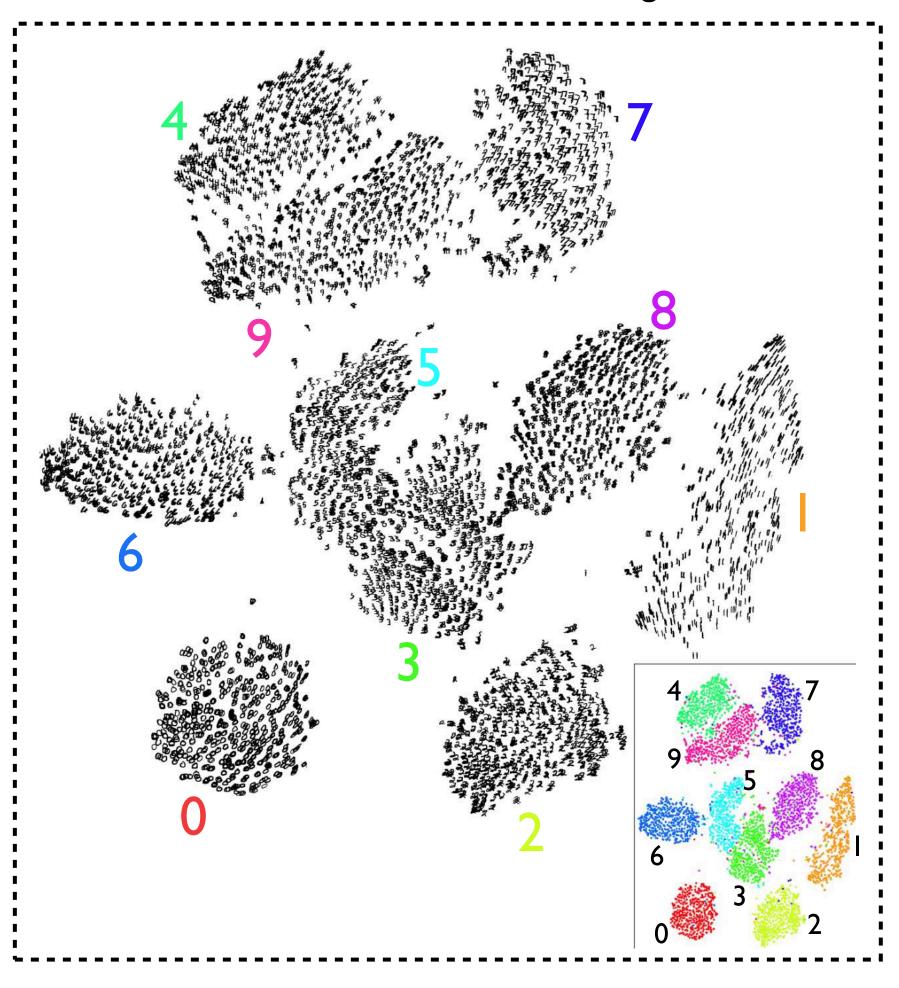
by soft and collinear limits

 \mathcal{U} Uniform event, not contained in any P_N

Visualizing Geometry in the Space of Events

t-Distributed Stochastic Neighbor Embedding (t-SNE)

MNIST handwritten digits

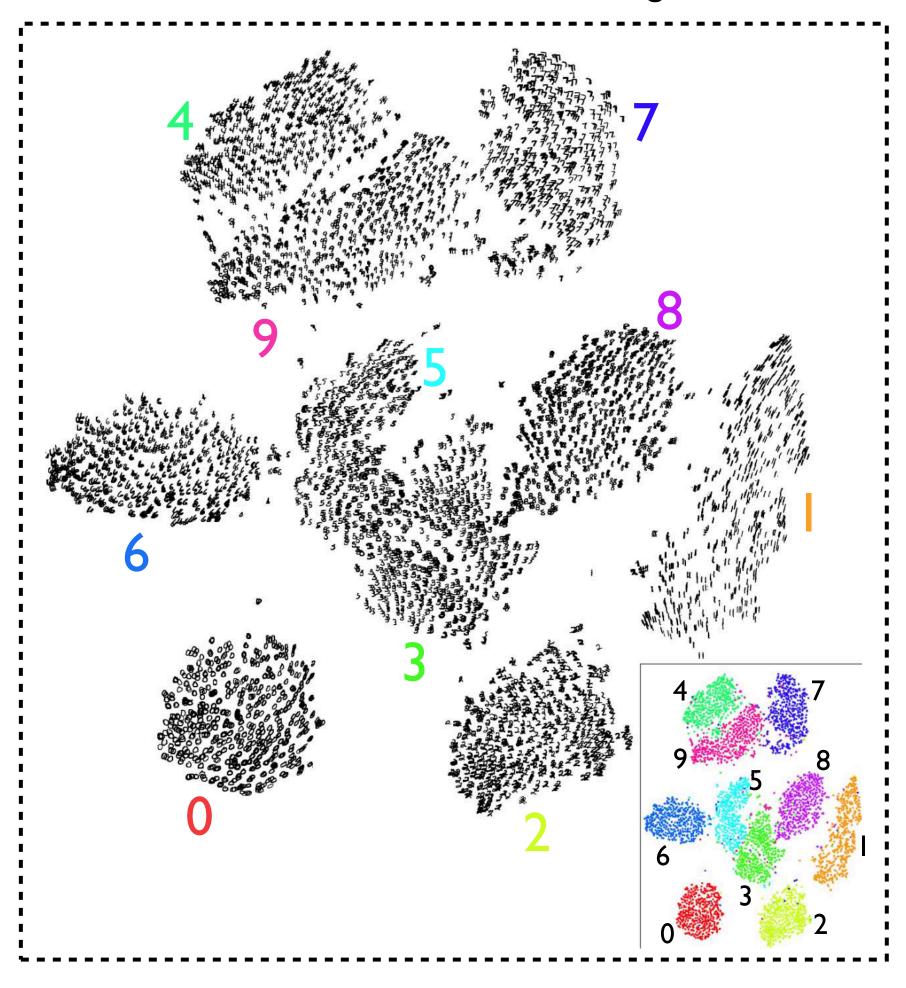


[L. van der Maaten, G. Hinton, JMLR 2008]

Visualizing Geometry in the Space of Events

t-Distributed Stochastic Neighbor Embedding (t-SNE)

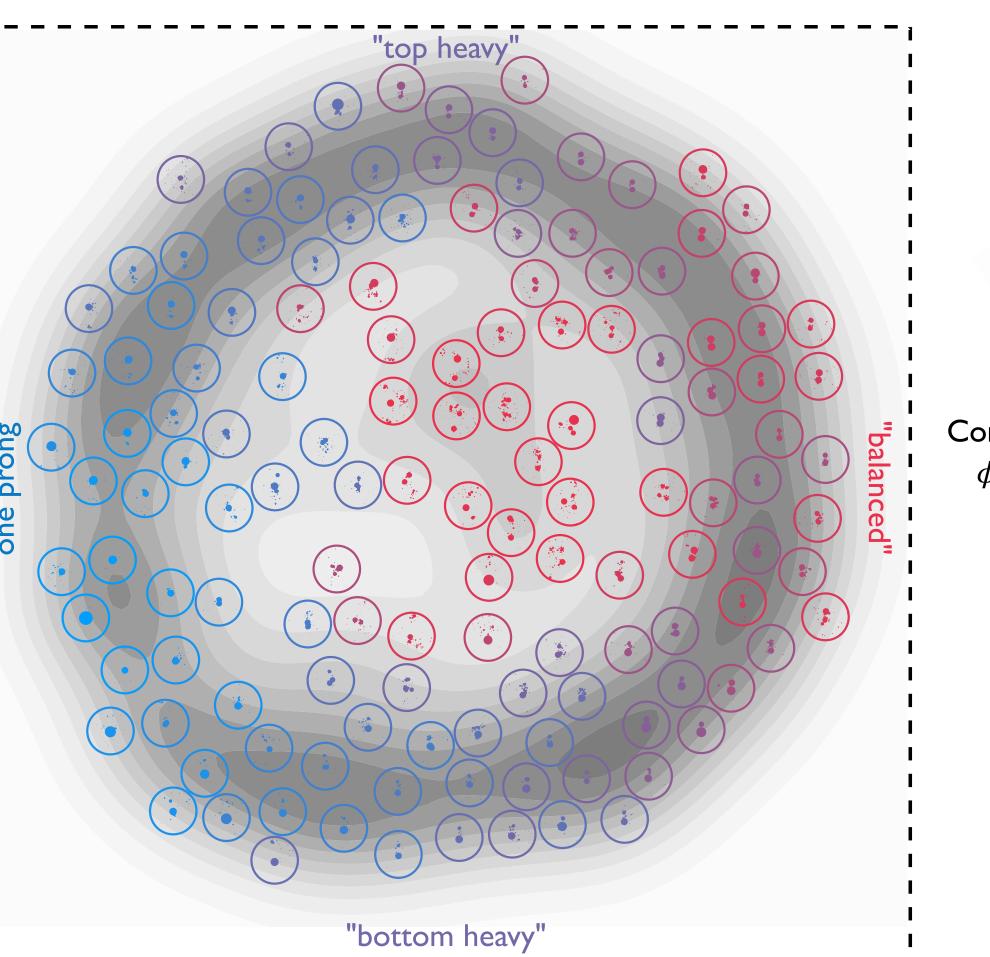
MNIST handwritten digits

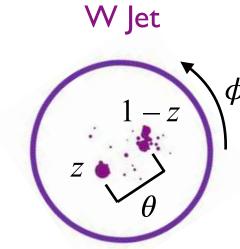


[L. van der Maaten, G. Hinton, JMLR 2008]

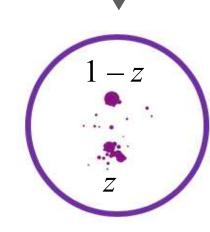
Geometric space of W jets

[PTK, Metodiev, Thaler, PRL 2019]





Constraints: W Mass and $\phi = 0$ preprocessing

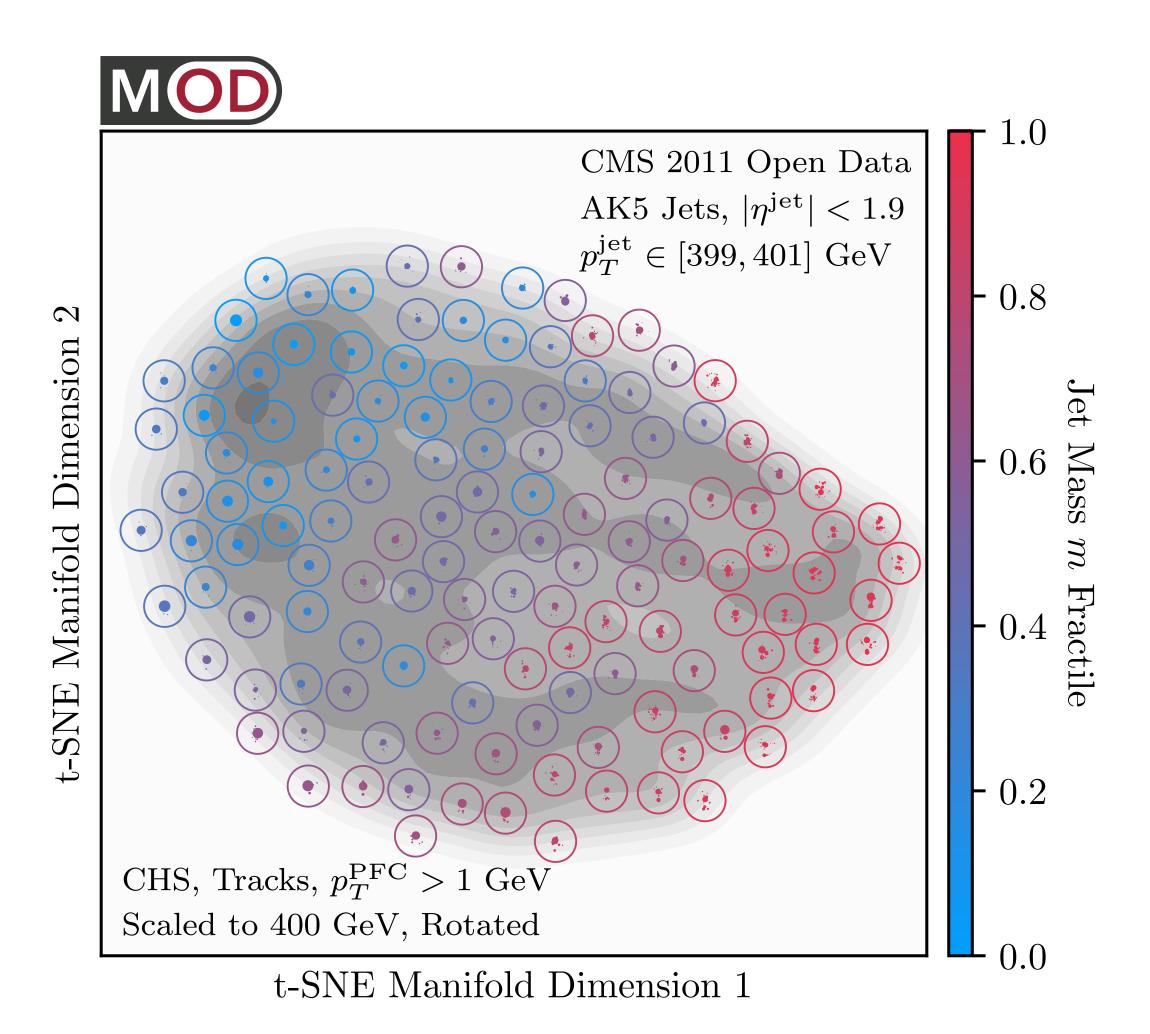


Gray contours represent the density of jets Each circle is a particular W jet

Visualizing Geometry in CMS Open Data



[PTK, Mastandrea, Metodiev, Naik, Thaler, PRD 2019; code and datasets at energyflow.network]

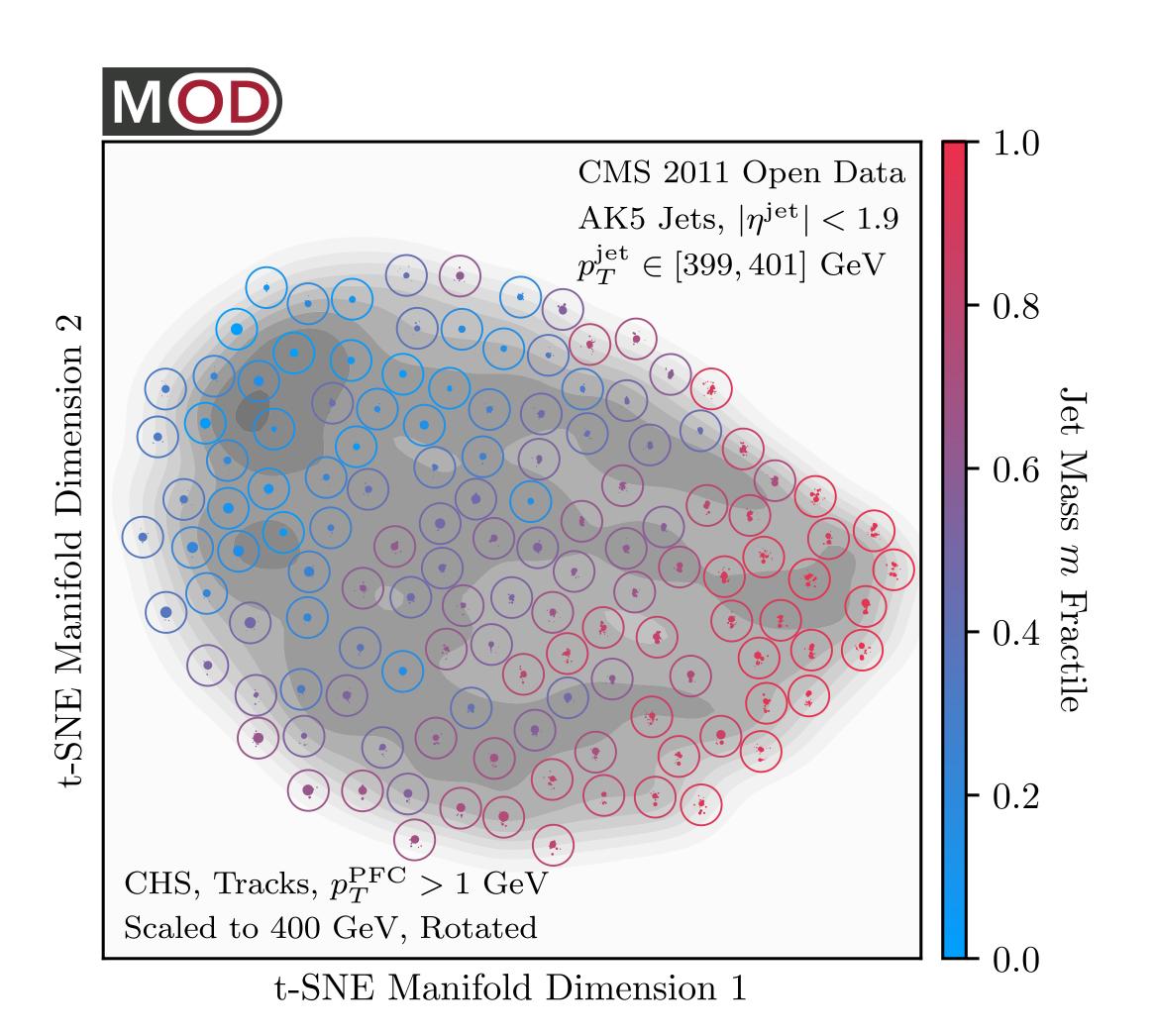


QCD produces mostly one-pronged jets but has long tails

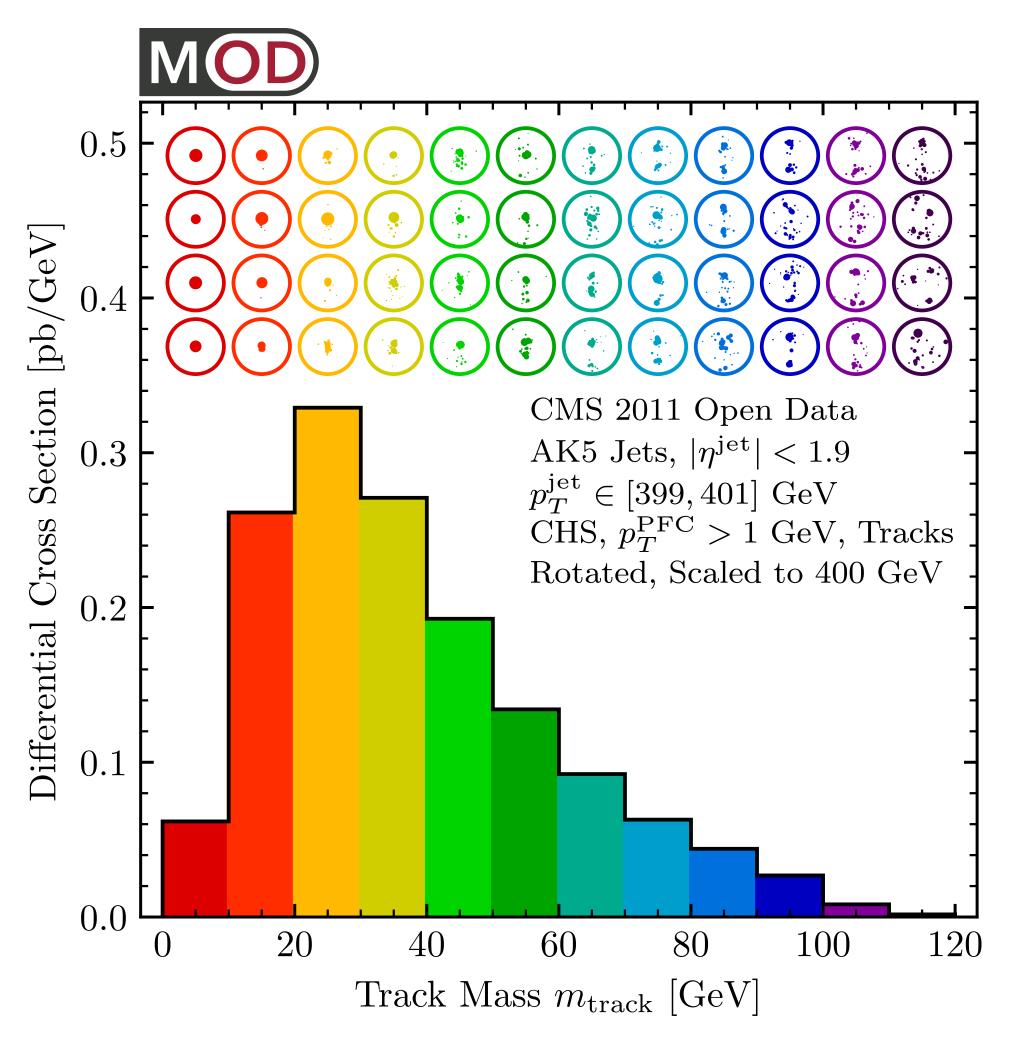
Visualizing Geometry in CMS Open Data



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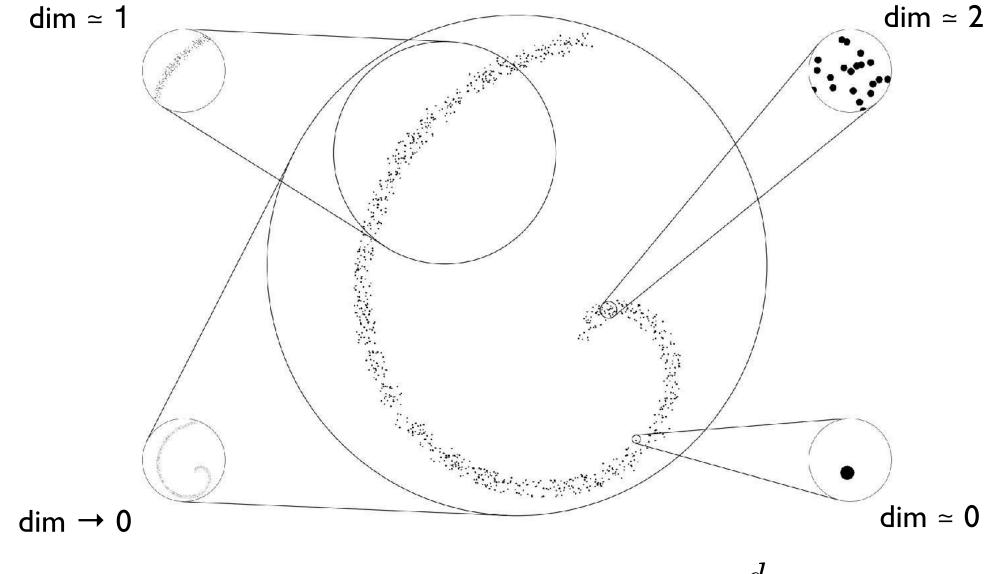


QCD produces mostly one-pronged jets but has long tails

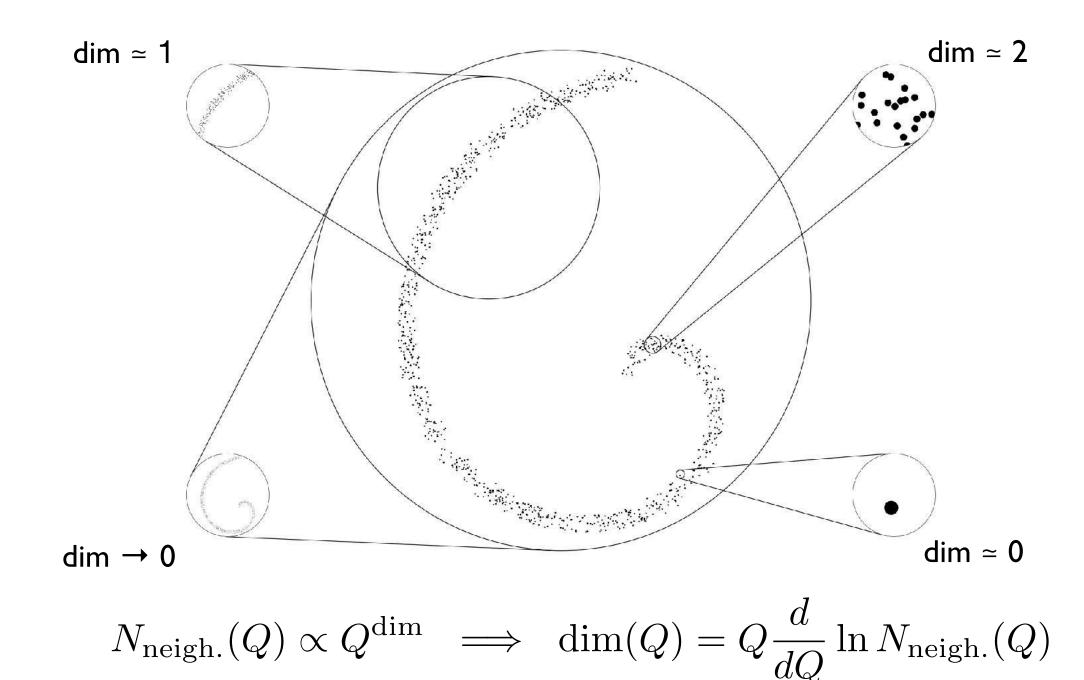


4 most representative jets (medoids) shown for each bin

Correlation dimension: how does the # of elements within a ball of size Q change?

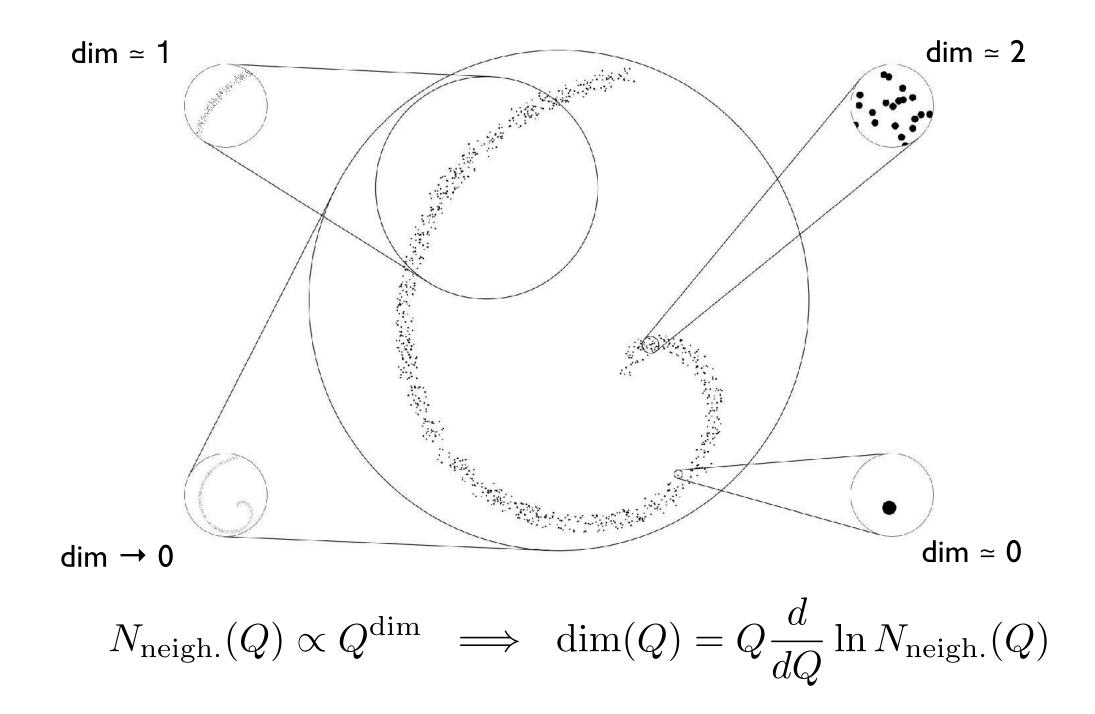


Correlation dimension: how does the # of elements within a ball of size Q change?



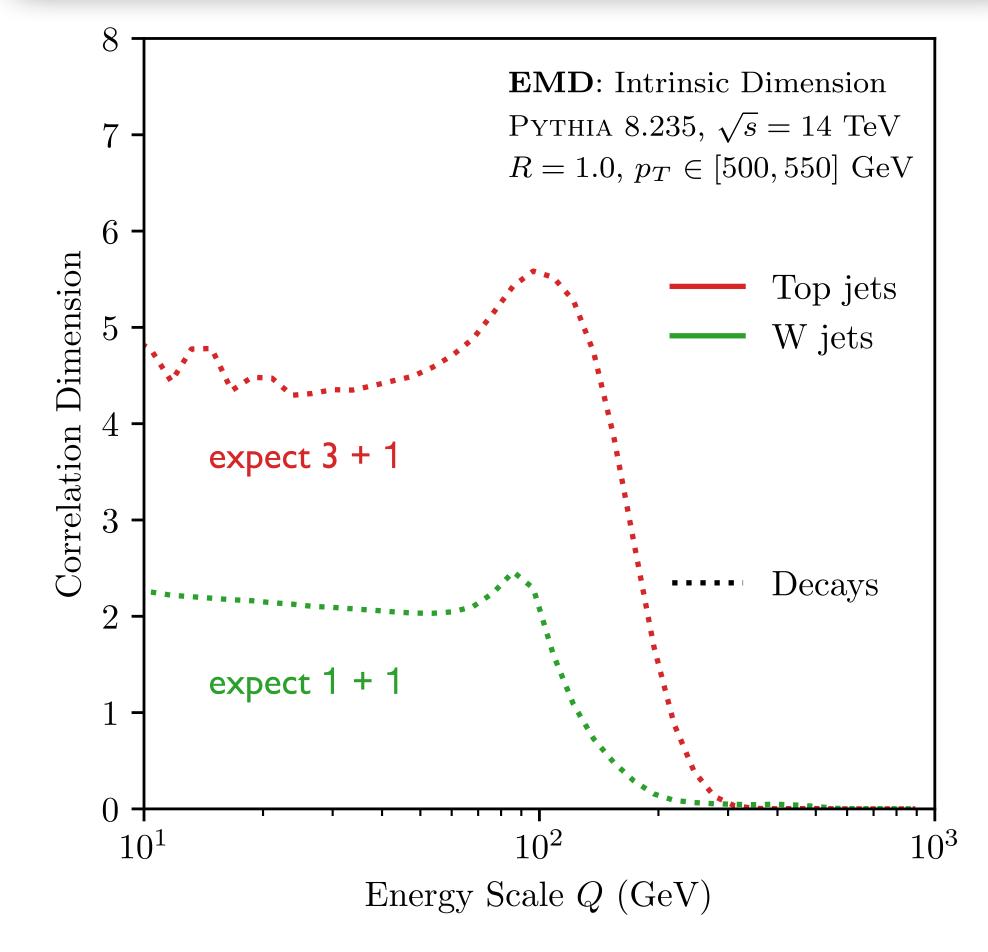
$$\dim(Q) = Q \frac{\partial}{\partial Q} \ln \sum_{i} \sum_{j} \Theta(\text{EMD}(\mathcal{E}_{i}, \mathcal{E}'_{j}) < Q)$$

Correlation dimension: how does the # of elements within a ball of size Q change?



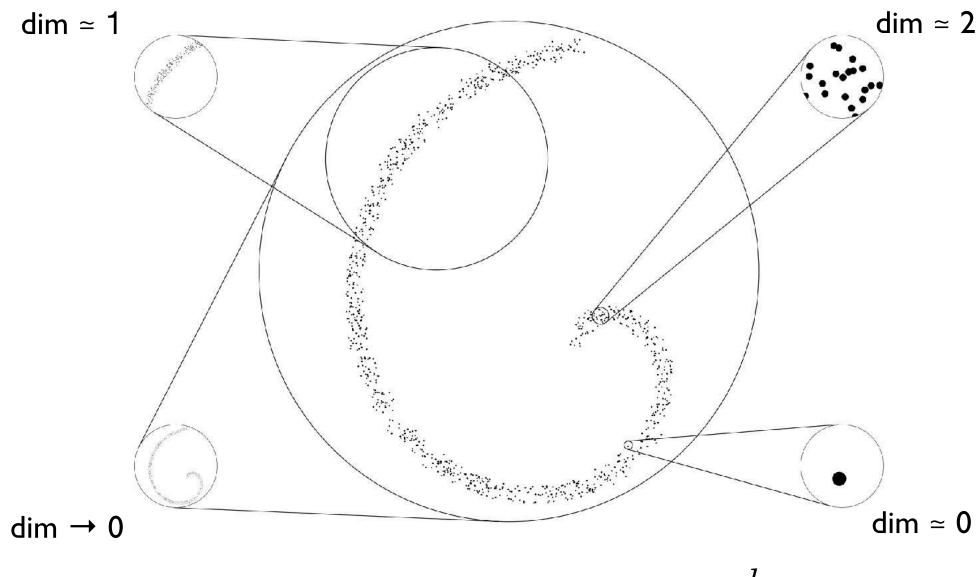
Correlation dimension lessons: Decays are "constant" dim. at low Q

$$\dim(Q) = Q \frac{\partial}{\partial Q} \ln \sum_{i} \sum_{j} \Theta(\text{EMD}(\mathcal{E}_{i}, \mathcal{E}'_{j}) < Q)$$



[Grassberger, Procaccia, PRL 1983; PTK, Metodiev, Thaler, PRL 2019]

Correlation dimension: how does the # of elements within a ball of size Q change?



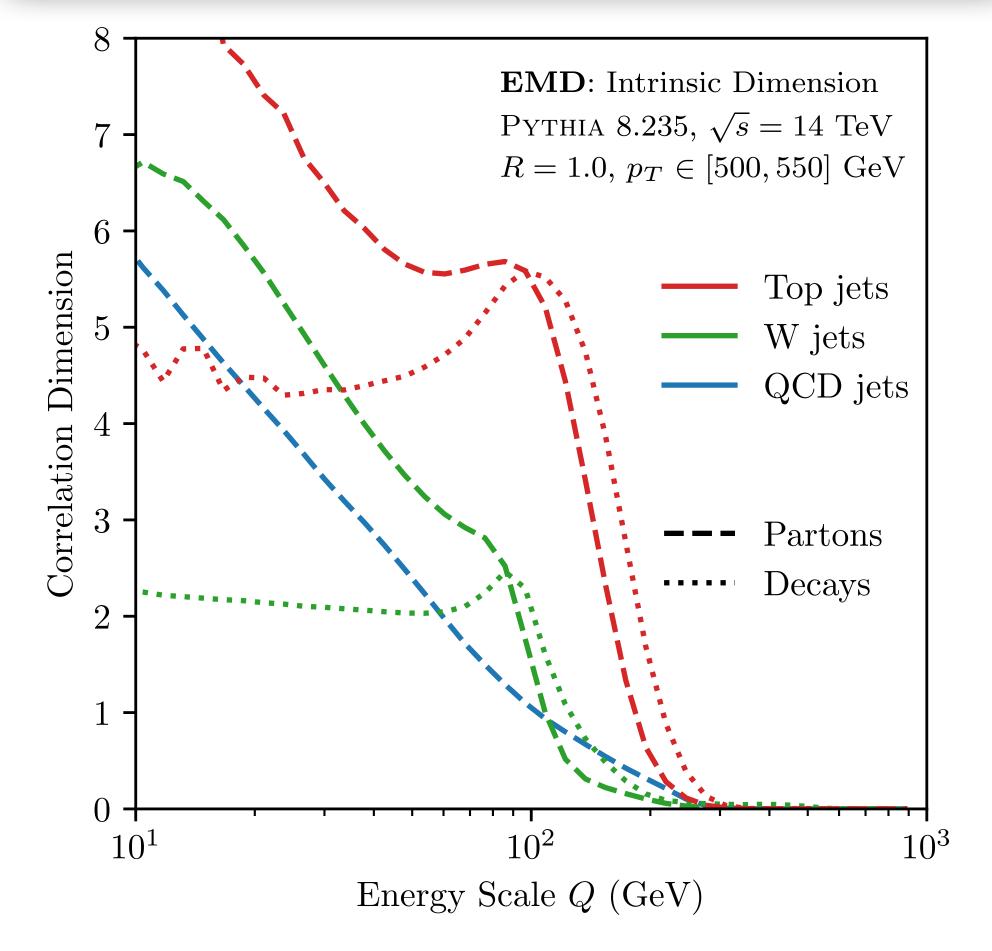
$$N_{\text{neigh.}}(Q) \propto Q^{\text{dim}} \implies \dim(Q) = Q \frac{d}{dQ} \ln N_{\text{neigh.}}(Q)$$

Correlation dimension lessons:

Decays are "constant" dim. at low *Q*Complexity hierarchy: QCD < W < Top

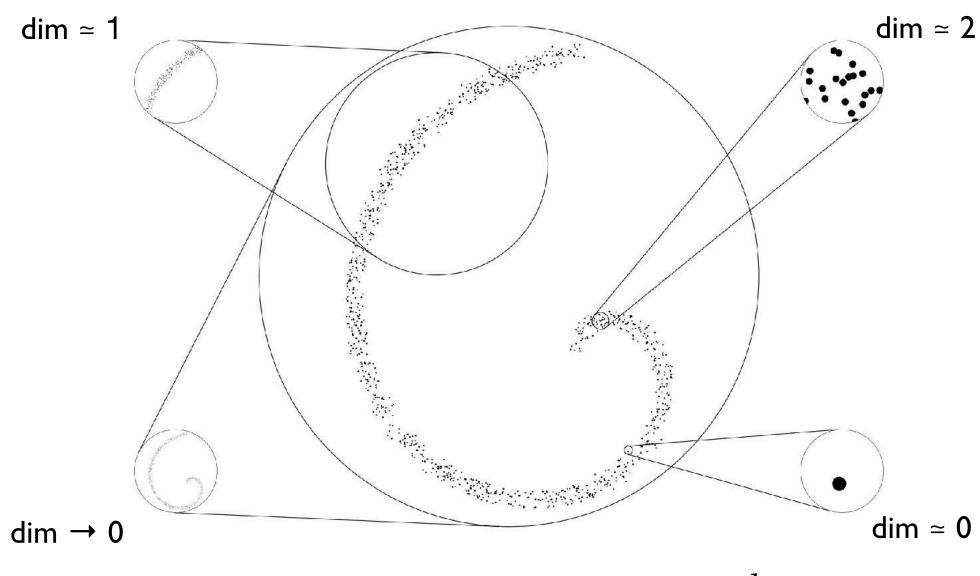
Fragmentation increases dim. at smaller scales

$$\dim(Q) = Q \frac{\partial}{\partial Q} \ln \sum_{i} \sum_{j} \Theta(\text{EMD}(\mathcal{E}_{i}, \mathcal{E}'_{j}) < Q)$$



[Grassberger, Procaccia, PRL 1983; PTK, Metodiev, Thaler, PRL 2019]

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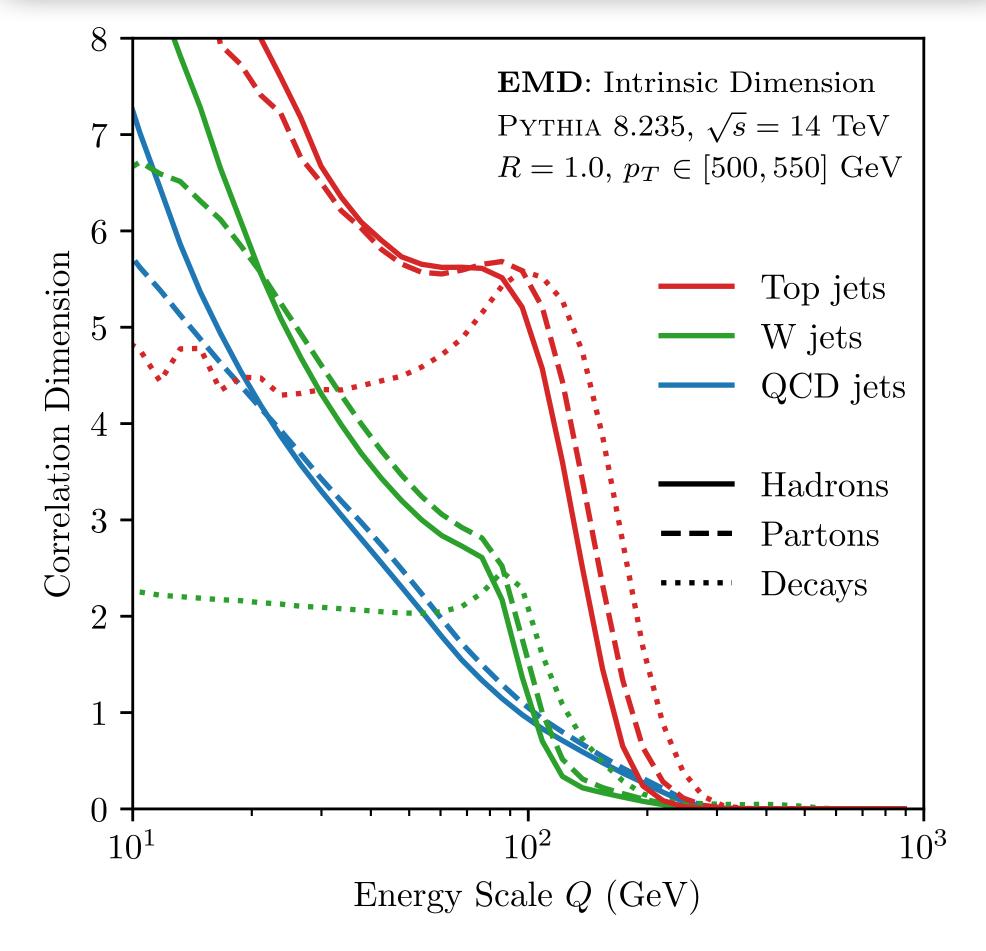


$$N_{\text{neigh.}}(Q) \propto Q^{\text{dim}} \implies \dim(Q) = Q \frac{d}{dQ} \ln N_{\text{neigh.}}(Q)$$

Correlation dimension lessons:

Decays are "constant" dim. at low *Q*Complexity hierarchy: QCD < W < Top
Fragmentation increases dim. at smaller scales
Hadronization important around 20-30 GeV

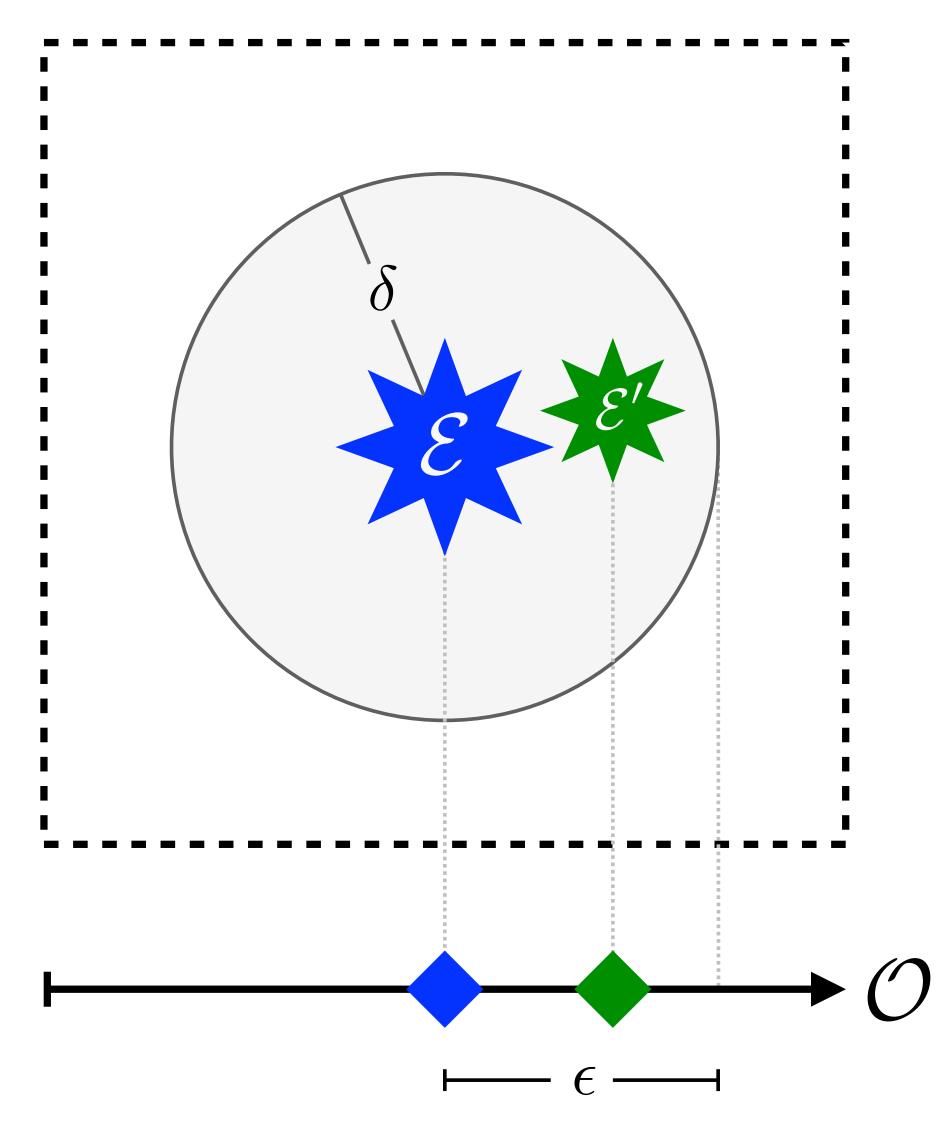
$$\dim(Q) = Q \frac{\partial}{\partial Q} \ln \sum_{i} \sum_{j} \Theta(\text{EMD}(\mathcal{E}_{i}, \mathcal{E}'_{j}) < Q)$$



[Grassberger, Procaccia, PRL 1983; PTK, Metodiev, Thaler, PRL 2019]

More EMD Geometry – Continuity in the Space of Events

[PTK, Metodiev, Thaler, 2004.04159]



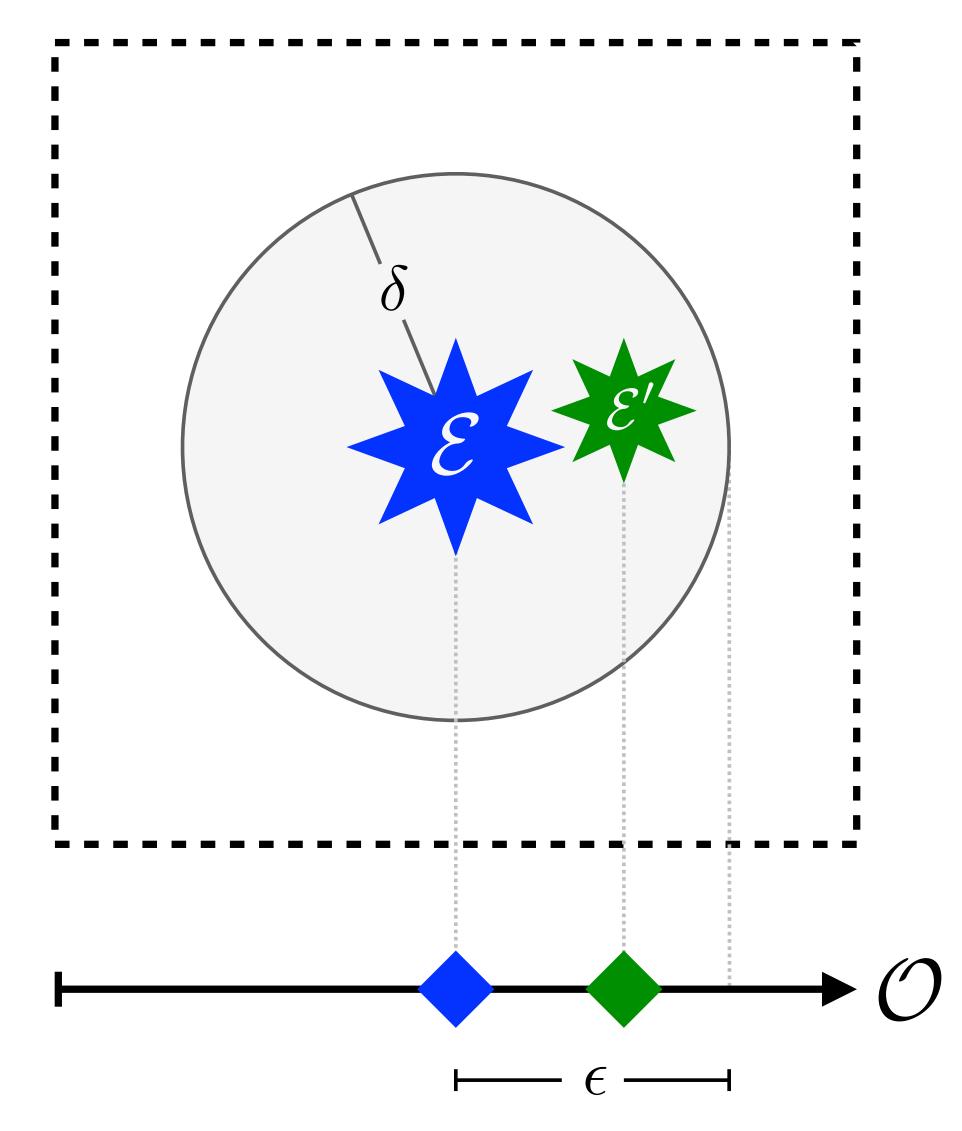
Classic $\epsilon - \delta$ definition of continuity in a metric space

An observable \mathcal{O} is EMD continuous at an event \mathcal{E} if, for any $\epsilon > 0$, there exists a $\delta > 0$ such that for all events \mathcal{E}' :

$$\mathrm{EMD}(\mathcal{E}, \mathcal{E}') < \delta \implies |\mathcal{O}(\mathcal{E}) - \mathcal{O}(\mathcal{E}')| < \epsilon.$$

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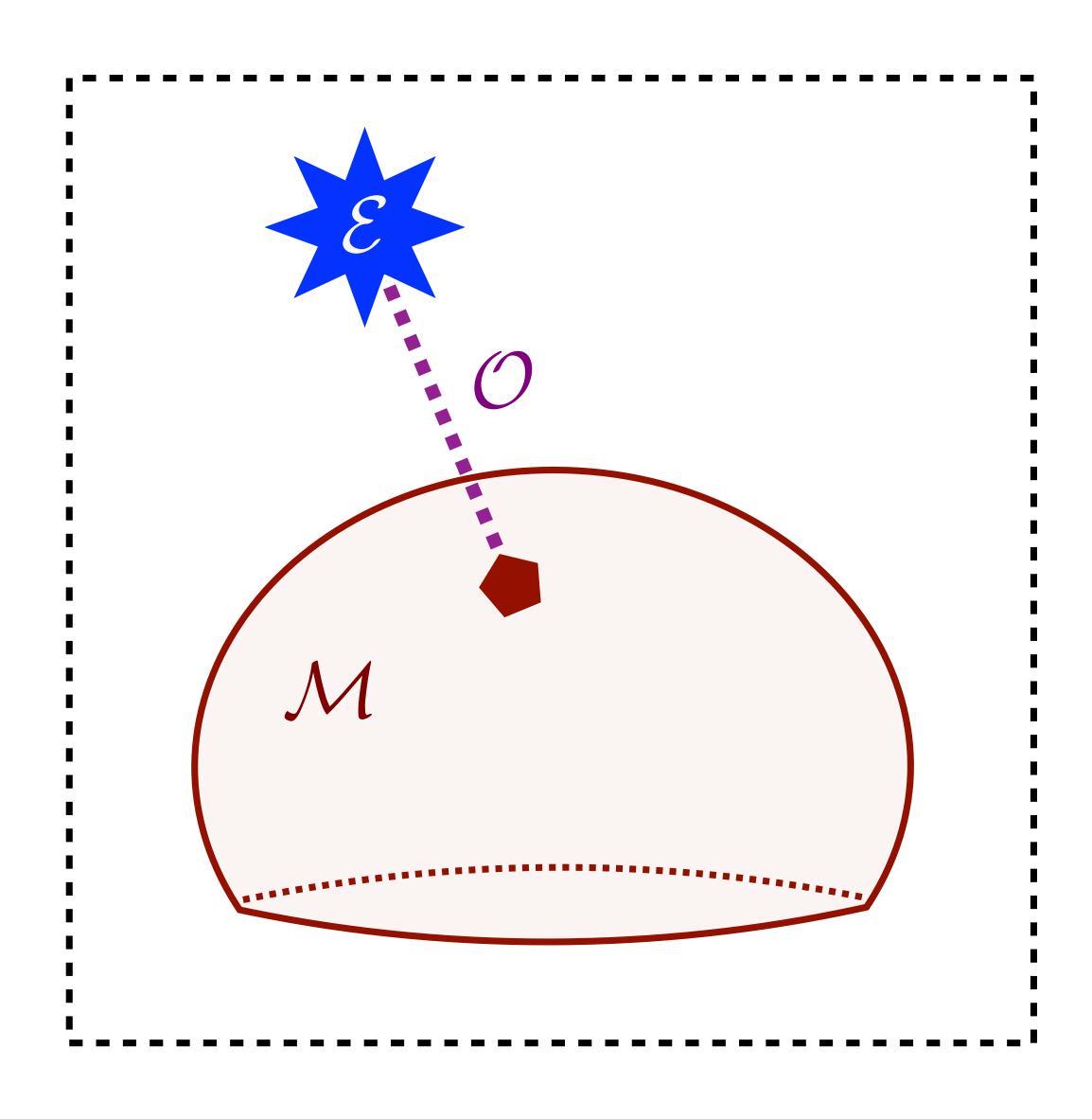
$$\mathrm{EMD}(\mathcal{E}, \mathcal{E}') < \delta \implies |\mathcal{O}(\mathcal{E}) - \mathcal{O}(\mathcal{E}')| < \epsilon.$$

Towards a geometric definition of IRC Safety

*on all but a negligible set‡ of events

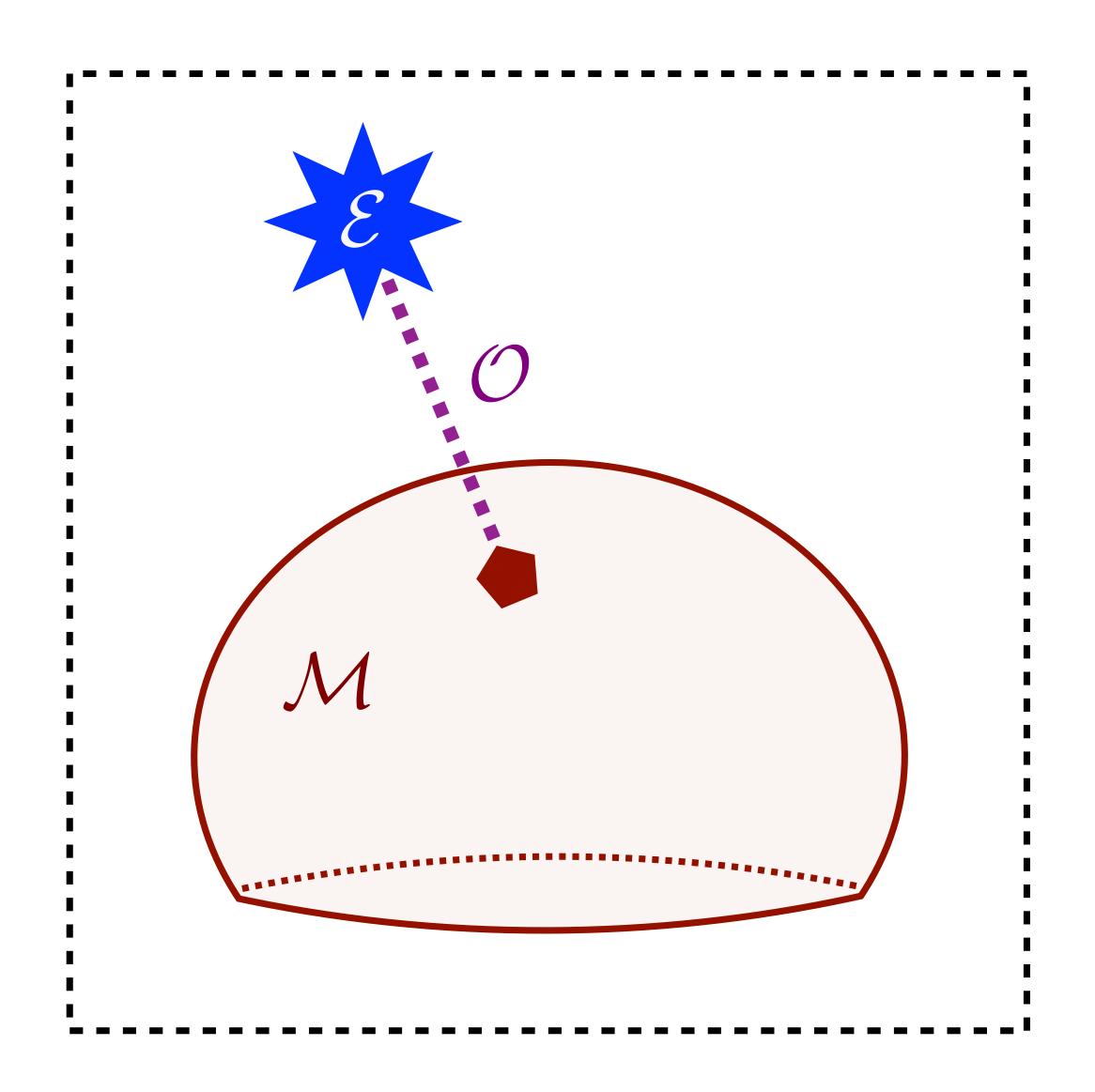
‡a negligible set is one that contains no positive-radius EMD-ball

•



Many common observables are distance of closest approach from event to a specific manifold

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



Many common observables are distance of closest approach from event to a specific manifold

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

EMD variant for equal-energy events

$$\begin{split} & \mathrm{EMD}_{\beta}(\mathcal{E}, \mathcal{E}') = \lim_{R \to \infty} R^{\beta} \mathrm{EMD}_{\beta, R}(\mathcal{E}, \mathcal{E}') = \min_{\{f_{ij} \geq 0\}} \sum_{i=1}^{M} \sum_{j=1}^{M'} f_{ij} \theta_{ij}^{\beta} \\ & \mathrm{Enforces\ equal\ energy\ (else\ infinity)} \end{split}$$



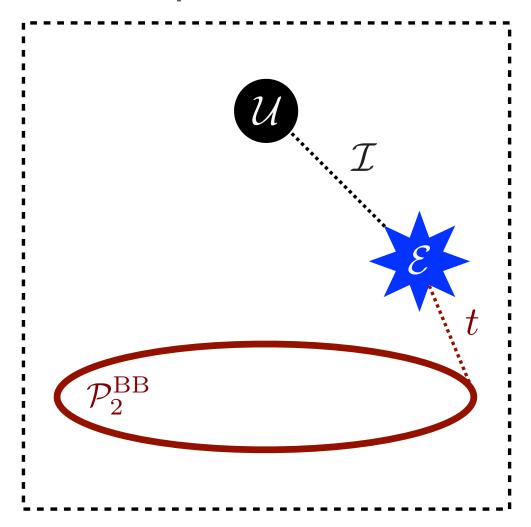
[PTK, Metodiev, Thaler, 2004.04159]



[PTK, Metodiev, Thaler, 2004.04159]

Thrust, spherocity, isotropy*

Distance of closest approach to a specific manifold



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

$$\sqrt{s(\mathcal{E})} = \min_{\mathcal{E}' \in \mathcal{P}_2^{\mathrm{BB}}} \mathrm{EMD}_1(\mathcal{E}, \mathcal{E}')$$

$$\mathcal{I}^{(\beta)}(\mathcal{E}) = \min_{\mathcal{E}' \in M_{\mathcal{U}}} \mathrm{EMD}_{\beta}(\mathcal{E}, \mathcal{E}')$$

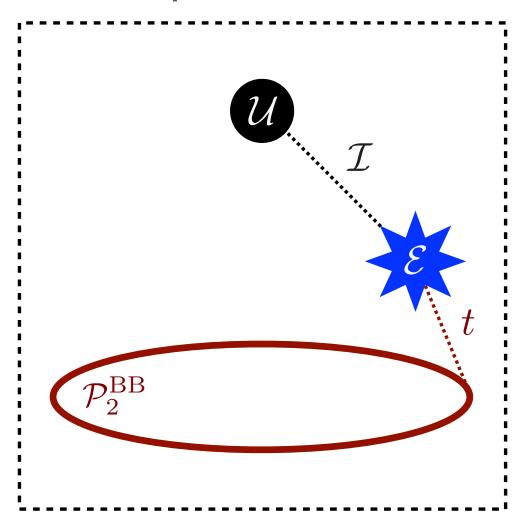
[Farhi, PRL 1977; Georgi, Machacek, PRL 1977]
*New! [Cesarotti, Thaler, 2004.06125]



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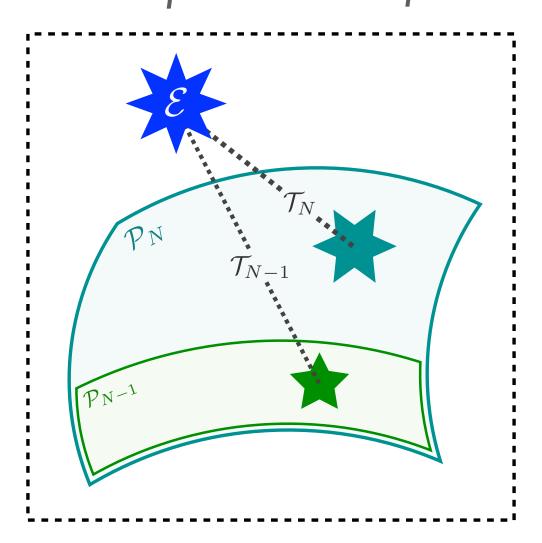
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[Farhi, PRL 1977; Georgi, Machacek, PRL 1977]
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N-jettiness

Minimum distance from event to N-particle manifold



without beam region

$$\mathcal{T}_N^{(\beta)}(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{P}_N} \mathrm{EMD}_{\beta}(\mathcal{E}, \mathcal{E}')$$

with constant beam distance R^{β}

$$\mathcal{T}_N^{(\beta,R)}(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{P}_N} \mathrm{EMD}_{\beta,R}(\mathcal{E}, \mathcal{E}')$$

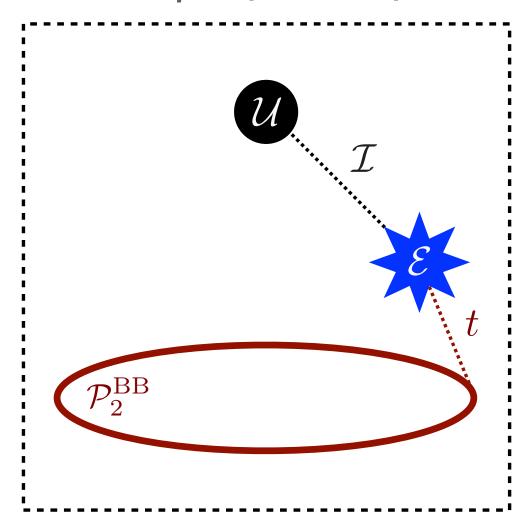
[Brandt, Dahmen, Z. Phys 1979; Stewart, Tackmann, Waalewijn, PRL 2010]



[PTK, Metodiev, Thaler, 2004.04159]

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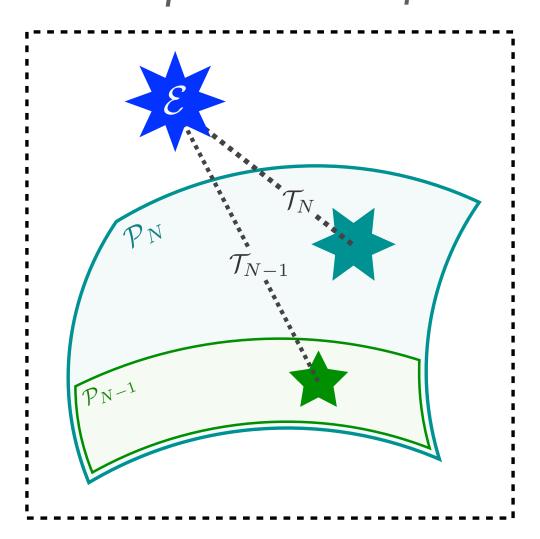
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*New! [Cesarotti, Thaler, 2004.06125]

N-jettiness

Minimum distance from event to N-particle manifold



without beam region

$$\mathcal{T}_N^{(eta)}(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{P}_N} \operatorname{EMD}_{eta}(\mathcal{E}, \mathcal{E}')$$

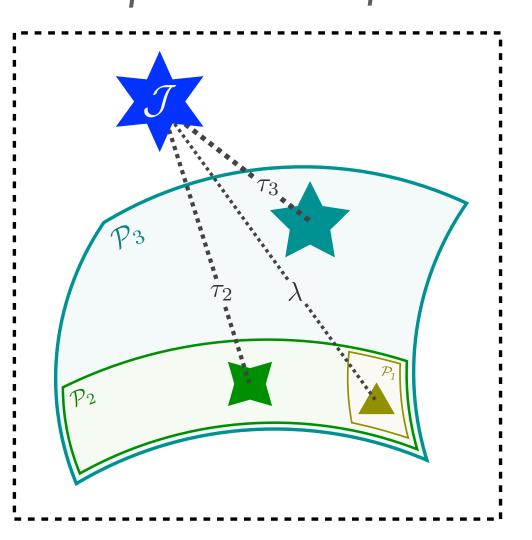
with constant beam distance R^{eta}

$$\mathcal{T}_N^{(\beta,R)}(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{P}_N} \mathrm{EMD}_{\beta,R}(\mathcal{E}, \mathcal{E}')$$

[Brandt, Dahmen, <u>Z. Phys 1979;</u> Stewart, Tackmann, Waalewijn, <u>PRL 2010</u>]

N-subjettiness, angularities

Smallest distance from jet to N-particle manifold



for recoil-free angularity

$$\lambda_{eta}(\mathcal{J}) = \min_{\mathcal{J}' \in \mathcal{P}_1} \mathrm{EMD}_{eta}(\mathcal{J}, \mathcal{J}')$$

$$au_N^{(eta)}(\mathcal{J}) = \min_{\mathcal{J}' \in \mathcal{P}_N} \mathrm{EMD}_{eta}(\mathcal{J}, \mathcal{J}')$$

[Ellis, Vermilion, Walsh, Hornig, Lee, JHEP 2010; Thaler, Van Tilburg, JHEP 2011, JHEP 2012]

Jets in the Space of Events – The Closest N-particle Description of an M-particle Event

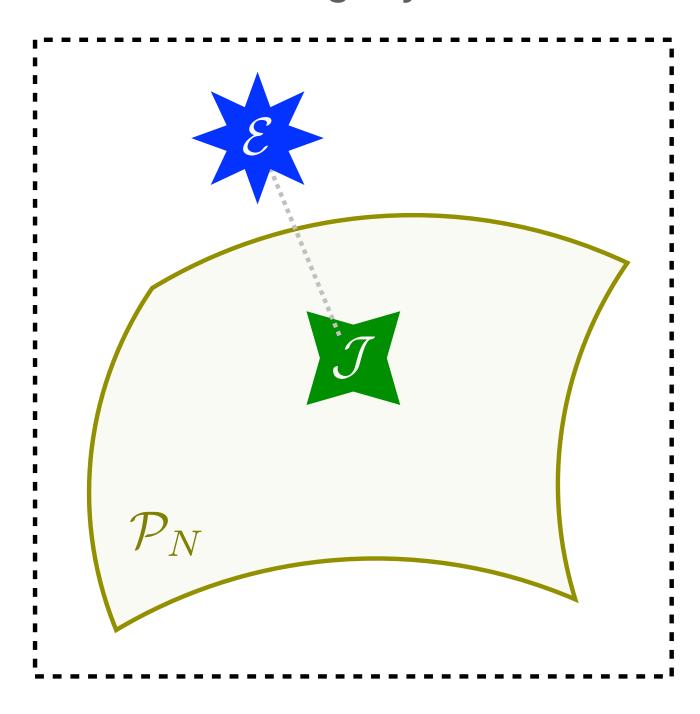
[PTK, Metodiev, Thaler, 2004.04159]

Jets in the Space of Events – The Closest N-particle Description of an M-particle Event

[PTK, Metodiev, Thaler, 2004.04159]

Exclusive cone finding

XCone finds N jets by minimizing N-jettiness



$$\mathcal{J}_{N,\beta,R}^{\text{XCone}}(\mathcal{E}) = \underset{\mathcal{J} \in \mathcal{P}_N}{\operatorname{arg\,min}\, \text{EMD}_{\beta,R}(\mathcal{E},\mathcal{J})}$$

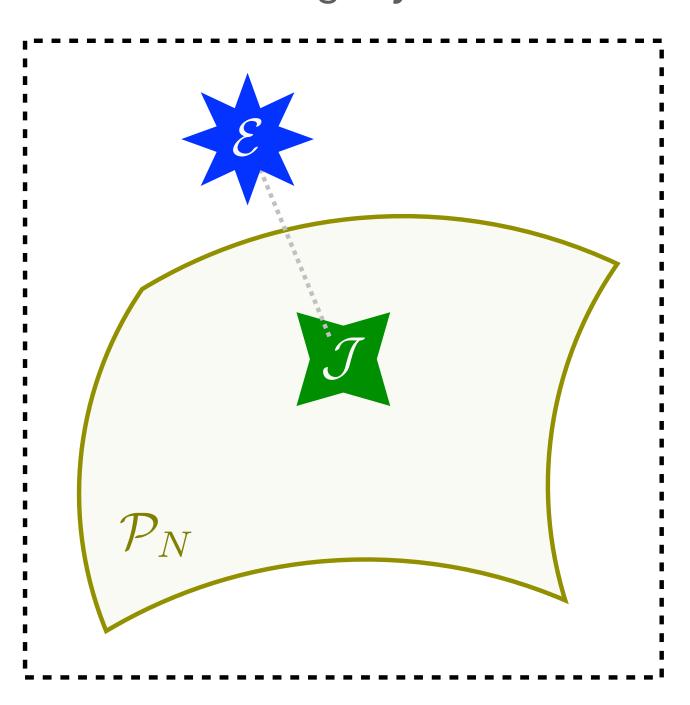
[Stewart, Tackmann, Thaler, Vermilion, Wilkason, JHEP 2015; Thaler, Wilkason, JHEP 2015]

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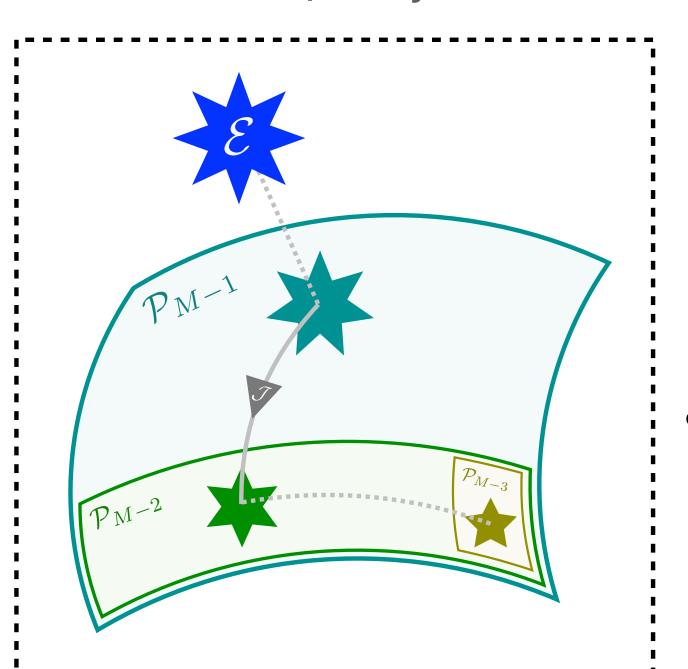


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[Stewart, Tackmann, Thaler, Vermilion, Wilkason, JHEP 2015; Thaler, Wilkason, JHEP 2015]

Sequential recombination

Iteratively merges particles or identifies a jet



"destroying" energy corresponds to identifying a jet

event with one fewer particle after one step

$$\mathcal{E}_{M-1}^{(\beta,R)}(\mathcal{E}_M) = \underset{\mathcal{E}'_{M-1} \in \mathcal{P}_{M-1}}{\operatorname{arg\,min}} \operatorname{EMD}_{\beta,R}(\mathcal{E}_M, \mathcal{E}'_{M-1})$$

[Catani, Dokshitzer, Seymour, Webber, Nucl. Phys. B 1993;

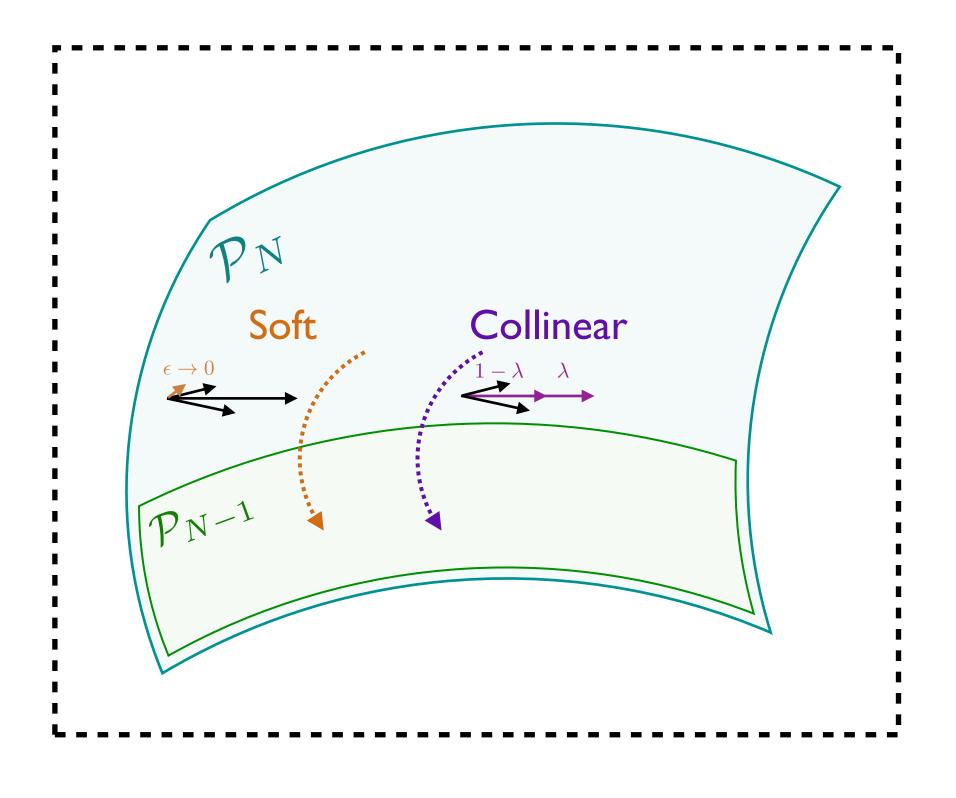
Ellis, Soper, PRD 1993;

Dokshitzer, Leder, Moretti, Webber, JHEP 1997;

Cacciari, Salam, Soyez, JHEP 2008]

[PTK, Metodiev, Thaler, 2004.04159]

Infrared singularities of massless gauge theories appear on each P_N



Perturbation Theory in the Space of Events

Sudakov safety

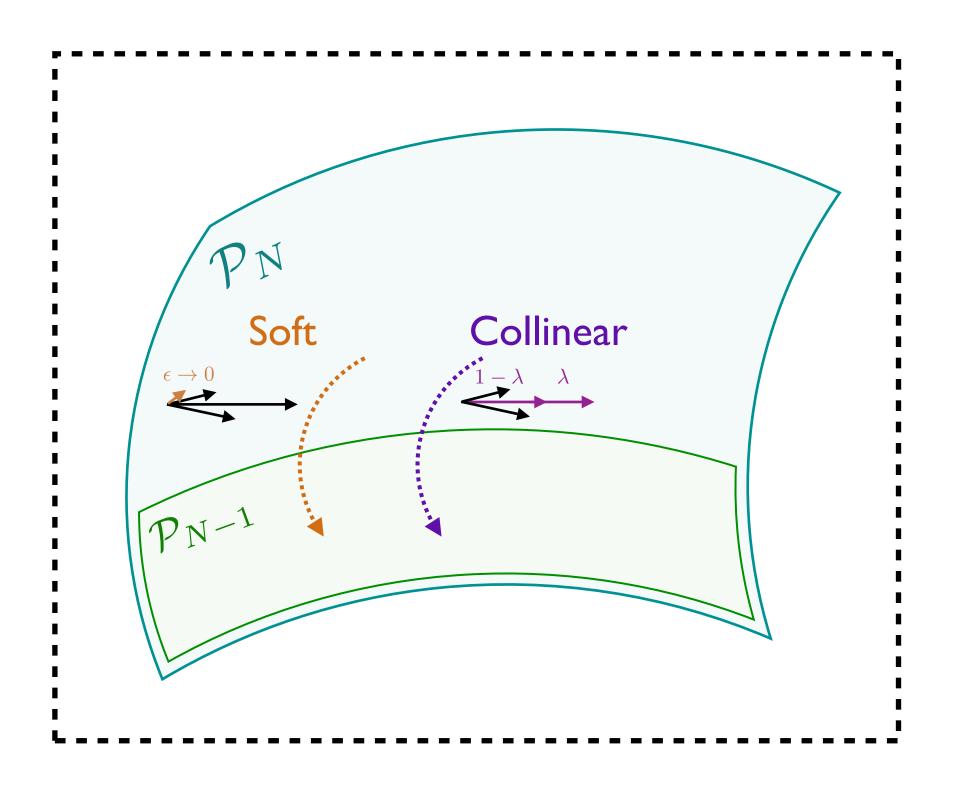
[Larkoski, Thaler, JHEP 2014; Larkoski, Marzani, Thaler, PRD 2015]

Some observables have discontinuities on P_N for some N A resummed IRC-safe companion can mitigate the divergences

$$p(\mathcal{O}_{\text{Sudakov}}) = \int d\mathcal{O}_{\text{Comp.}} p(\mathcal{O}_{\text{Sudakov}} | \mathcal{O}_{\text{Comp.}}) p(O_{\text{Comp.}})$$

Event geometry suggests N-(sub)jettiness as universal companion

Infrared singularities of massless gauge theories appear on each P_N



Perturbation Theory in the Space of Events

Sudakov safety

[Larkoski, Thaler, JHEP 2014; Larkoski, Marzani, Thaler, PRD 2015]

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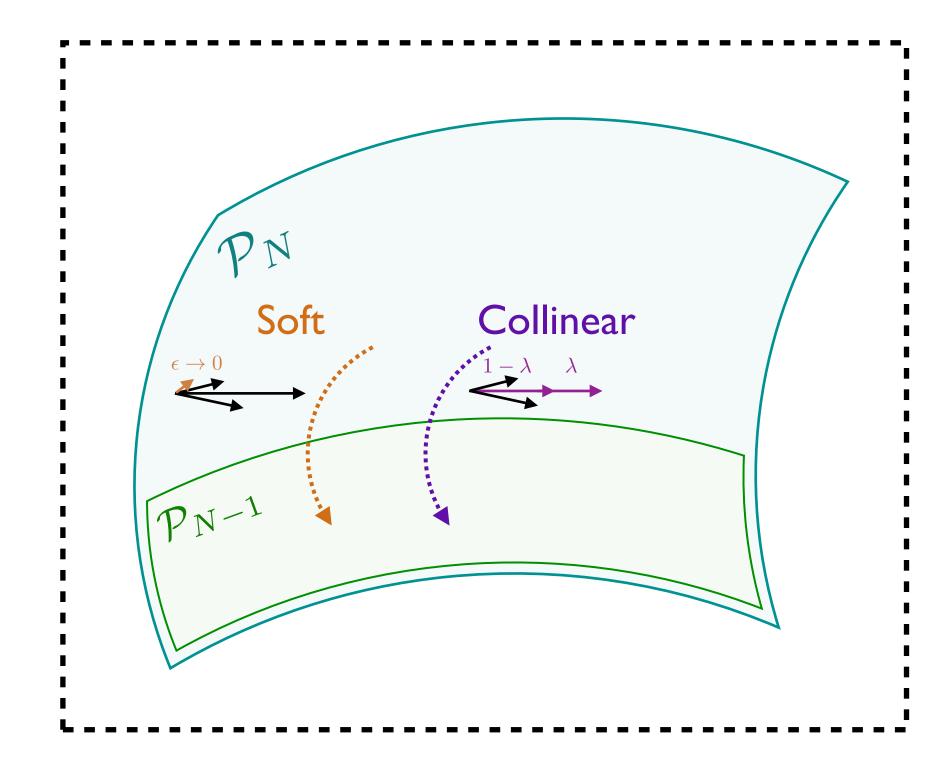
Fixed-order calculability

[Sterman, PRD 1979; Banfi, Salam, Zanderighi, JHEP 2005]

Is a statement of integrability on each P_N EMD continuity must be upgraded to EMD-Hölder continuity on each P_N

$$\lim_{\mathcal{E} \to \mathcal{E}'} \frac{\mathcal{O}(\mathcal{E}) - \mathcal{O}(\mathcal{E}')}{\text{EMD}(\mathcal{E}, \mathcal{E}')^c} = 0, \quad c > 0$$

Infrared singularities of massless gauge theories appear on each P_N



Example: $V(\mathcal{E}) = \mathcal{T}_2(\mathcal{E}) \left(1 + \frac{1}{\ln E(\mathcal{E})/\mathcal{T}_3(\mathcal{E})} \right)$ is EMD continuous but not EMD Hölder continuous (it is Sudakov safe)

Hierarchy of IRC Safety Definitions

[PTK, Metodiev, Thaler, 2004.04159]

All Observables

Measurable at a collider

Defined on Energy Flows

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

Infrared & Collinear Safe

EMD continuous everywhere except a negligible set of events

EMD Hölder Continuous

Everywhere invariant to infinitesimal infrared & collinear emissions

Sudakov Safe

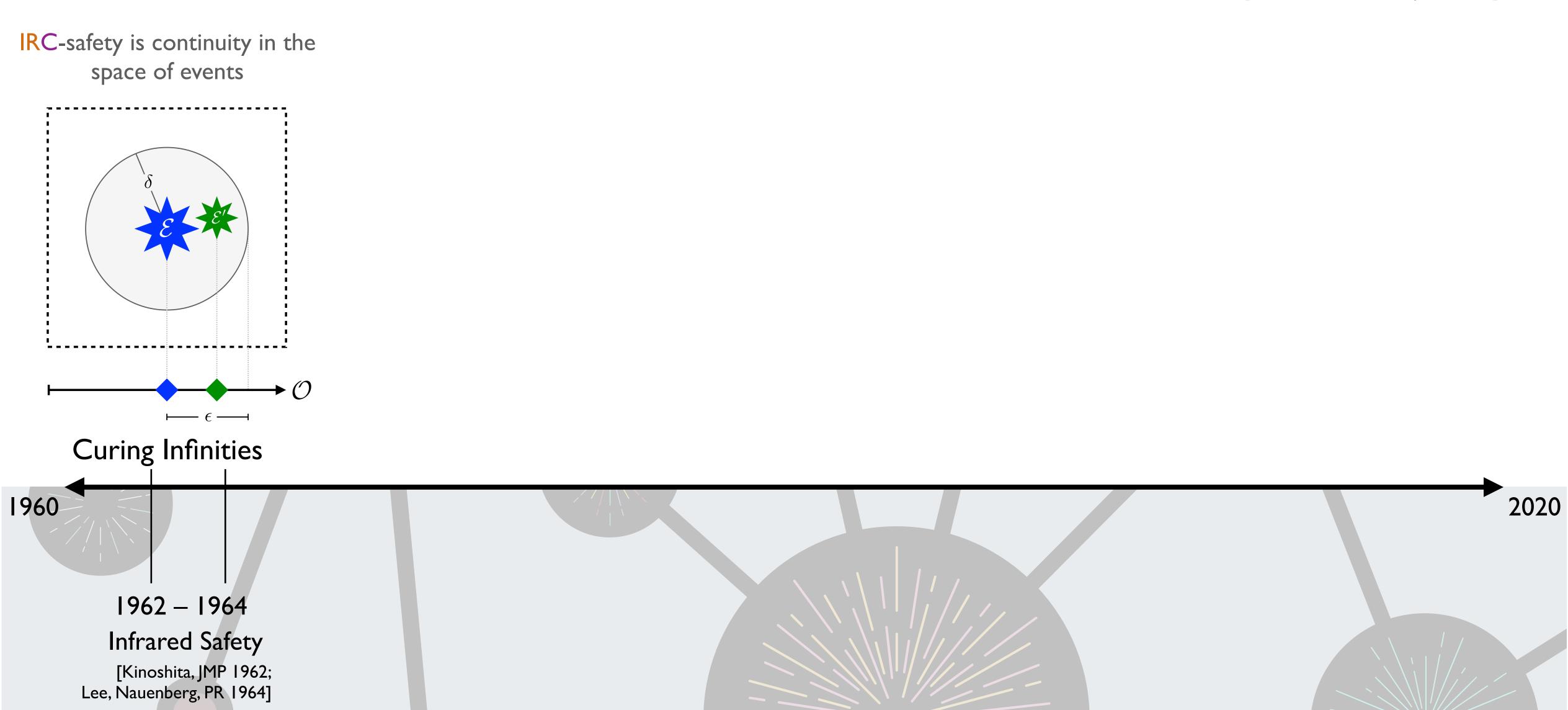
Discontinuous on some N-particle manifolds

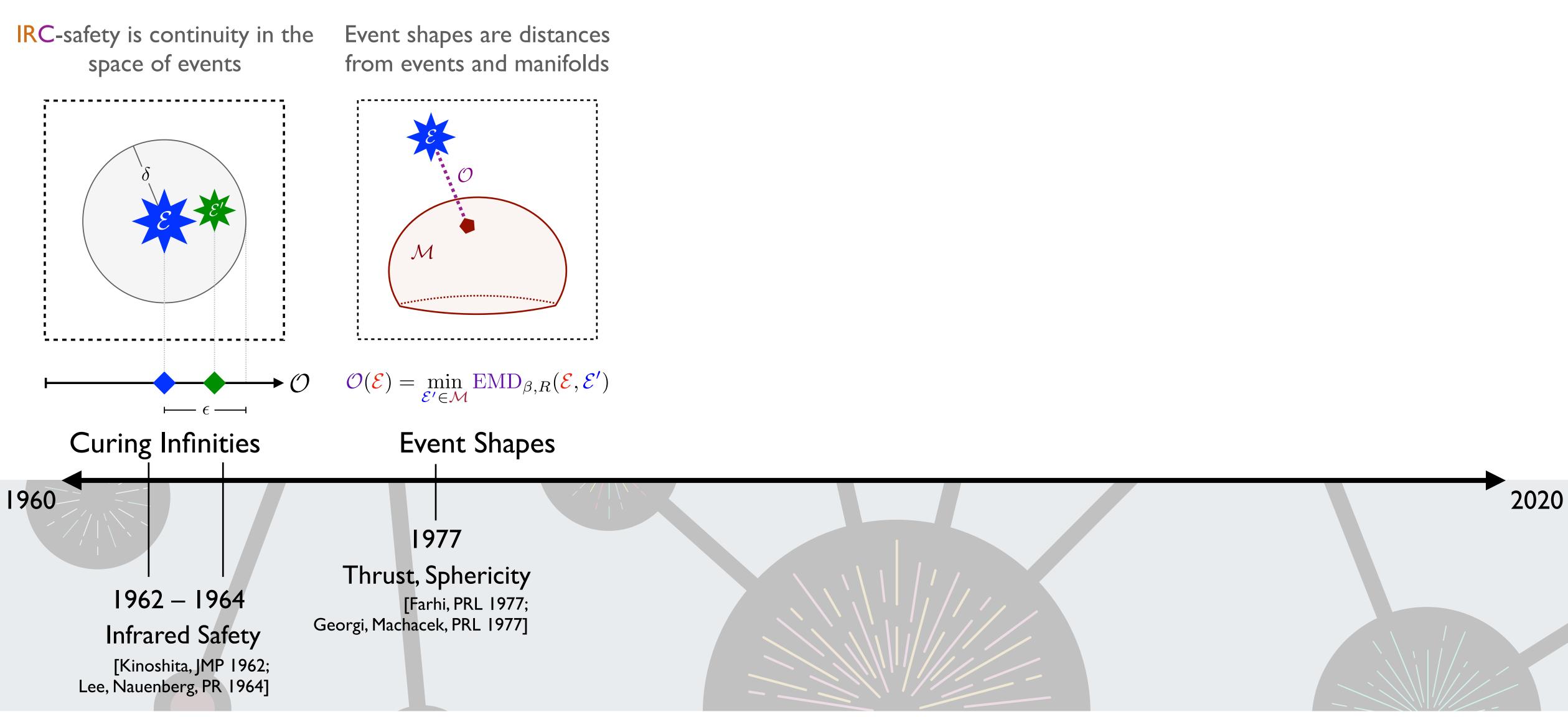
All	Observables	Comments		
Multiplicity $(\sum_i 1)$		IR unsafe and C unsafe		
Momentum Dispersion [65] $(\sum_i E_i^2)$		IR safe but C unsafe		
Sphericity Tensor [66] $(\sum_i p_i^{\mu} p_i^{\nu})$		IR safe but C unsafe		
Nu	mber of Non-Zero Calorimeter Deposits	C safe but IR unsafe		
	Defined on Energy Flows			
	Pseudo-Multiplicity (min $\{N \mid \mathcal{T}_N = 0\}$)	Robust to exact IR or C emissions		

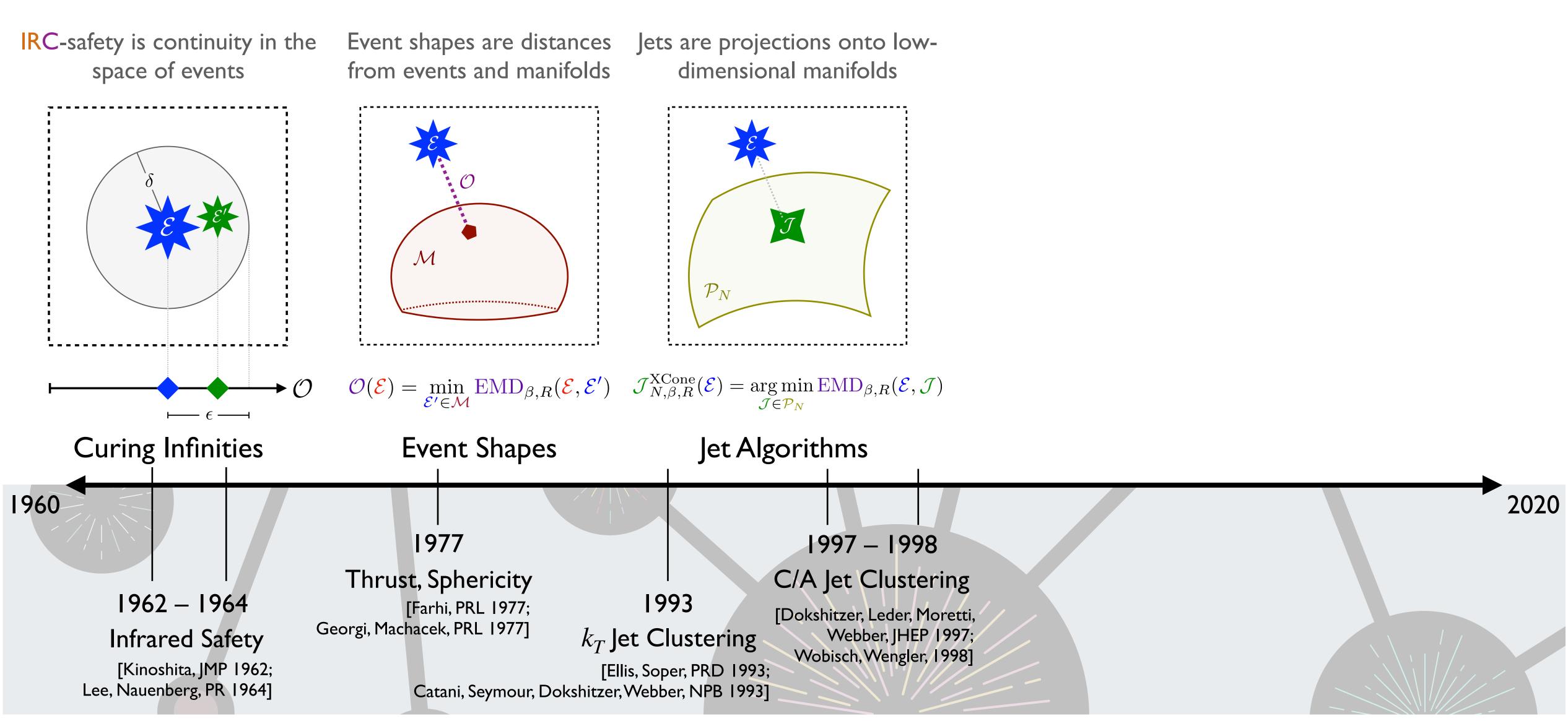
seudo-Multiplicity (min{ $N \mid J_N = 0$ })	Robust to exact IR or C emissions			
Infrared & Collinear Safe				
Jet Energy $(\sum_i E_i)$	Disc. at jet boundary			
Heavy Jet Mass [67]	Disc. at hemisphere boundary			
Soft-Dropped Jet Mass [38, 68]	Disc. at grooming threshold			
Calorimeter Activity [69] (N_{95})	Disc. at cell boundary			
$Sudakov\ Safe$				
Groomed Momentum Fraction [39] (z_g)	Disc. on 1-particle manifold			
Jet Angularity Ratios [37]	Disc. on 1-particle manifold			
N -subjettiness Ratios [47, 48] (τ_{N+1}/τ_N)	Disc. on N -particle manifold			
V parameter [36] (Eq. (2.11))	Hölder disc. on 3-particle manifold			

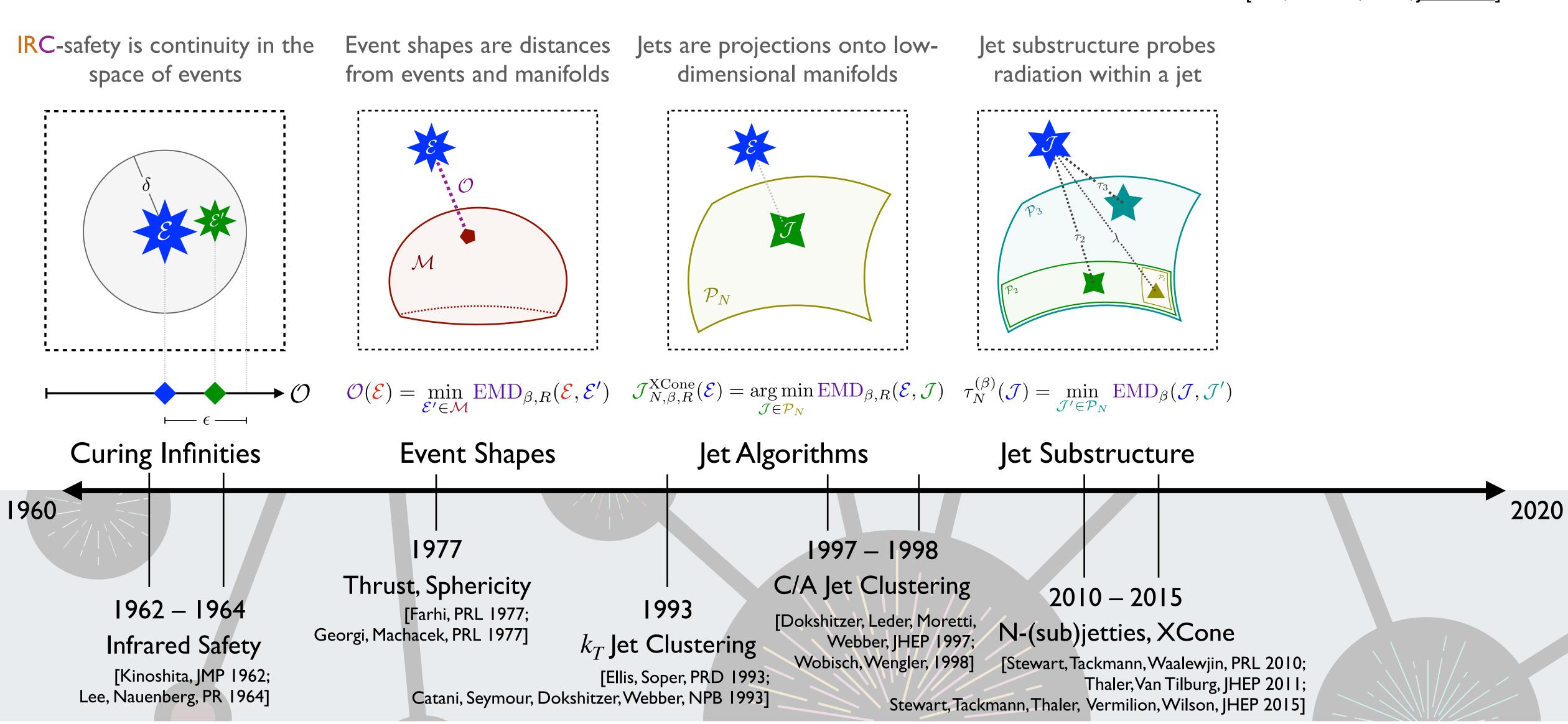
EMD Hölder Continuous Everywhere Thrust [40, 41] Spherocity [42] Angularities [70] N-jettiness [44] (\mathcal{T}_N) C parameter [71–74] Linear Sphericity [72] ($\sum_i E_i n_i^{\mu} n_i^{\nu}$) Energy Correlators [36, 75–77] Energy Flow Polynomials [15, 17]











Catani, Seymour, Dokshitzer, Webber, NPB 1993]

IRC-safety is continuity in the Event shapes are distances Jets are projections onto low-Jet substructure probes Pileup mitigation moves away from events and manifolds dimensional manifolds from the uniform event space of events radiation within a jet $\mathcal{J}_{N,\beta,R}^{\text{XCone}}(\mathcal{E}) = \underset{\mathcal{J} \in \mathcal{P}_N}{\operatorname{arg\,min}} \operatorname{EMD}_{\beta,R}(\mathcal{E},\mathcal{J}) \quad \tau_N^{(\beta)}(\mathcal{J}) = \underset{\mathcal{J}' \in \mathcal{P}_N}{\operatorname{min}} \operatorname{EMD}_{\beta}(\mathcal{J},\mathcal{J}')$ $\mathcal{O}(\mathcal{E}) = \min_{\mathcal{E}' \in \mathcal{M}} \mathrm{EMD}_{\beta, R}(\mathcal{E}, \mathcal{E}')$ $\mathcal{E}_C(\mathcal{E}, \rho) = \underset{\mathcal{E}' \in \Omega}{\operatorname{arg \, min}} \ \mathrm{EMD}_{\beta}(\mathcal{E}, \mathcal{E}' + \rho \, \mathcal{U})$ Curing Infinities Event Shapes Jet Algorithms Jet Substructure Pileup Subtraction 1960 2020 1977 1997 - 19982014 - 2019Thrust, Sphericity C/A Jet Clustering Constituent Subtraction 2010 - 20151962 - 19641993 [Farhi, PRL 1977; [Berta, Spousta, Miller, Leitner, JHEP 2014; [Dokshitzer, Leder, Moretti, N-(sub)jetties, XCone Georgi, Machacek, PRL 1977] Berta, Masetti, Miller, Spousta, JHEP 2019] Webber, JHEP 1997; k_T Jet Clustering Infrared Safety Wobisch, Wengler, 1998] [Stewart, Tackmann, Waalewjin, PRL 2010; [Kinoshita, JMP 1962; [Ellis, Soper, PRD 1993; Thaler, Van Tilburg, JHEP 2011;

Lee, Nauenberg, PR 1964]

Stewart, Tackmann, Thaler, Vermilion, Wilson, JHEP 2015]