Modeling of hadronization

Andrzej Siódmok Jagiellonian University



https://indico.cern.ch/event/1176398

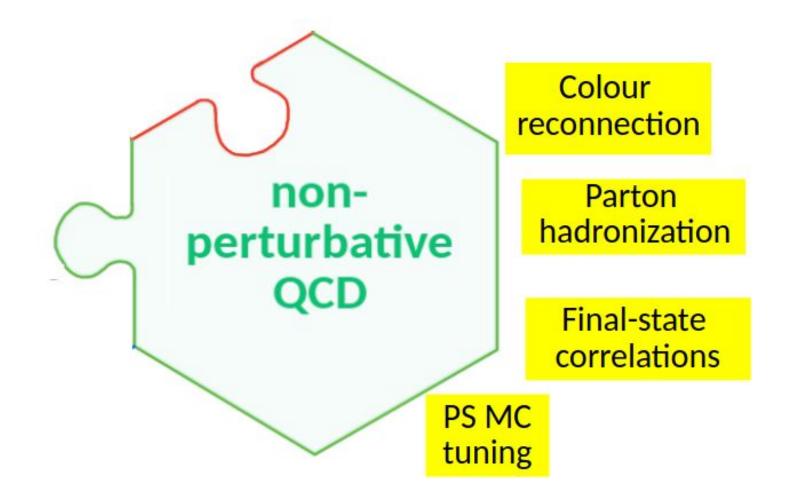


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Outline



Thanks to David d'Enterria

Motivation - Monte Carlo Event Generators (MCEG)

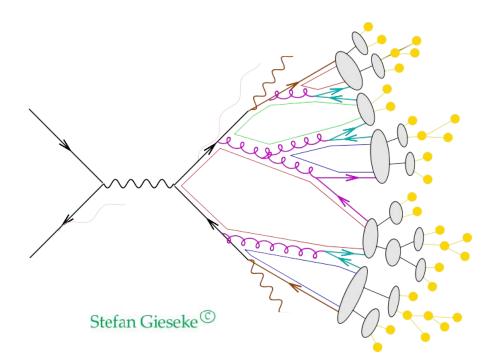
QCD correctly describes strong interactions in each energy range but its complex mathematical structure makes it very difficult to obtain precise predictions (Millennium Prize Problem \$1,000,000)

High energy

- perturbative QCD
- in theory we know what to do
- in practice very difficult

Low energy

- non-perturbative QCD
- we don't know what to do
- phenomenological models (with many free parameters)



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Motivation - Monte Carlo Event Generators (MCEG)

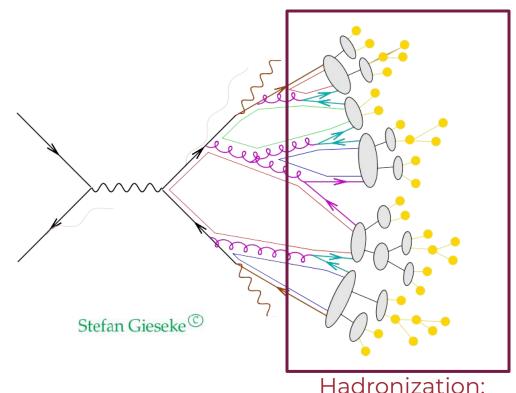
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one of the least understood elements of MCEG

Motivation - Hadronization

Hadronization:

- → Increased control of perturbative corrections ⇒ more often LHC measurements are limited by non-perturbative components, such as hadronization.
 - W mass measurement using a new method [Freytsis at al. JHEP 1902 (2019) 003]
 - Extraction of the strong coupling in [M. Johnson, D. Maître, Phys.Rev. D97 (2018) no.5]
 - Top mass [S. Argyropoulos, T. Sjöstrand, JHEP 1411 (2014) 043]
 - ...

Pier Moni's talk

 However, hadronisation remains the main bottleneck 10^{2} Hgg [Gao '16] Hbb $\left| \sigma d\sigma / d(1-T) \right|$ e.g. thrust in Higgs decays (MC variation in plot) Hqq 10^{1} HWW Zaa 10⁰ Increase in energy insufficient for suppression ($Q \sim m_{H}$) 10^{-1} Runs at lower energies are essential for 10^{-2} a robust tuning of NP models in MCs e+e-, 250 GeV and 5 ab^{-1} 10^{-3} Thrust Also crucial for training of ML ∆^{th.unc.}(Hgg) ren.scale + hadronization 1.4 algorithms for jet tagging, instrumental = mat. scale 1.2 in extraction of Higgs couplings 1.0 0.8 0.6 0.1 0.2 0.3 0.4 0.5 0.0

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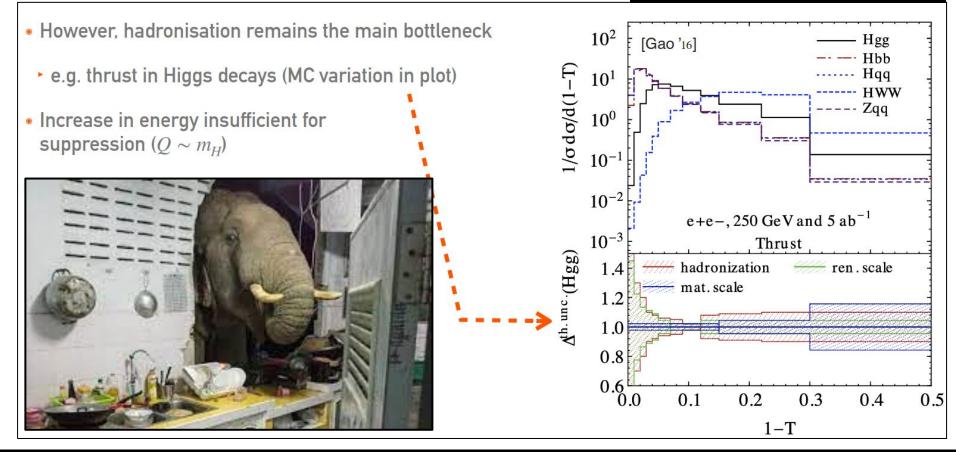
1-T

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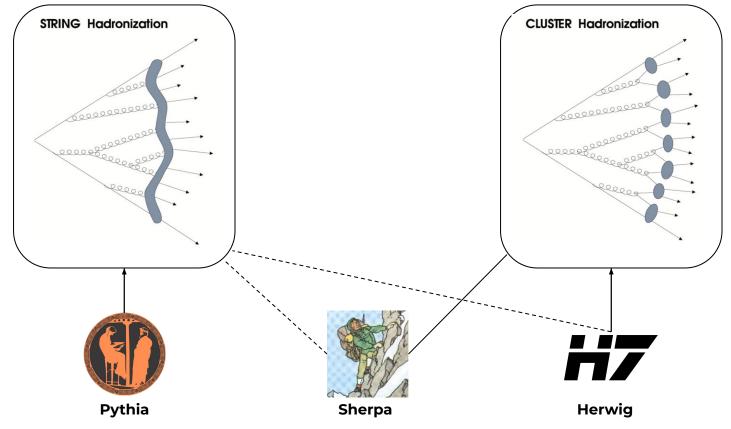


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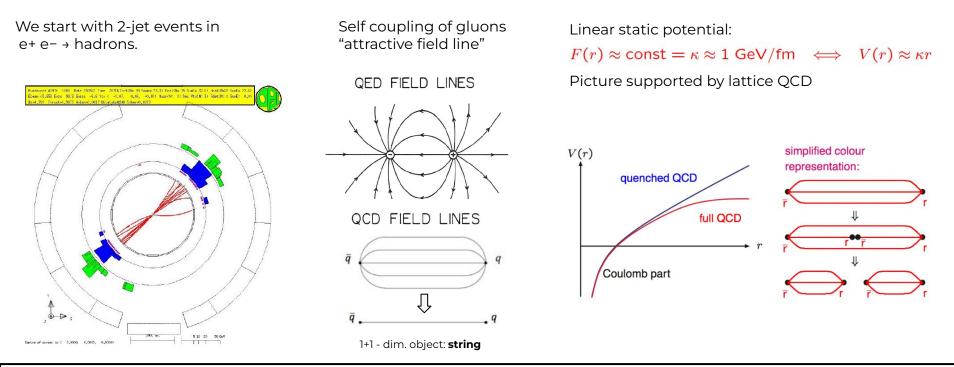
Motivation - Hadronization

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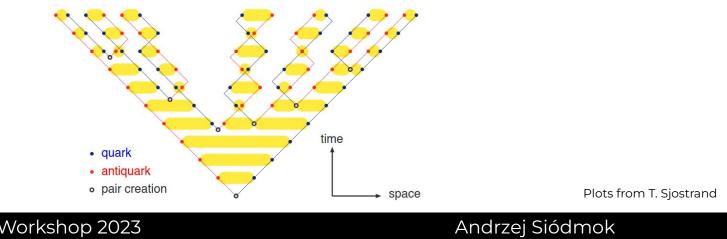
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 - ..



Originally invented without perturbative physics of parton showers in mind.



Lund string model: like rubber band that is pulled apart and breaks into pieces



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String Model in nutshell

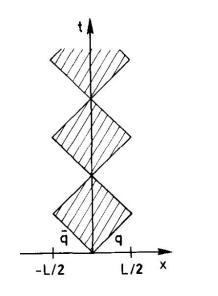
[Andersson, Gustafson, Ingelman, Sjostrand, Phys.Rept.97(1983)31]

String motion

From linear static potential $V(r) \approx \kappa r$ and linearity between space-time and energy-momentum:

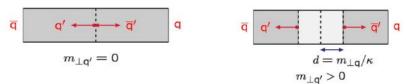
$$\left| \frac{\mathrm{d}E}{\mathrm{d}z} \right| = \left| \frac{\mathrm{d}p_z}{\mathrm{d}z} \right| = \left| \frac{\mathrm{d}E}{\mathrm{d}t} \right| = \left| \frac{\mathrm{d}p_z}{\mathrm{d}t} \right| = \kappa$$

We get a "YoYo" state which we interpret as a meson.



String breakdowns

The quarks obtain a mass and a transverse momentum in the breakup through a tunneling mechanism



with a probability:

$$\mathcal{P} \propto \exp\left(-\frac{\pi m_{\perp \mathbf{q}}^2}{\kappa}\right) = \exp\left(-\frac{\pi p_{\perp \mathbf{q}}^2}{\kappa}\right) \, \exp\left(-\frac{\pi m_{\mathbf{q}}^2}{\kappa}\right)$$

- Suppression of heavy quarks: uu : dd : ss : cc ≈ 1 : 1 : 0.3 : 10⁻¹¹
- Common Gaussian pT spectrum, <pT>~ 0.4 GeV
- Diquark (qq q̄q̄ breakups) ~ antiquark
 ⇒ simple model for baryon production.

Iterative process (left-right symmetry) leads to distribution of momentum fraction taken by each hadron as: $(1 - \alpha)^a - (-hm^2)$

$$f(z) \propto \frac{(1-z)^a}{z} \exp\left(-\frac{bm^2}{z}\right)$$

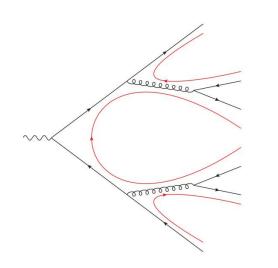
Summary:

String model has very good energy-momentum picture however it is unpredictive in understanding of hadron mass effects \Rightarrow many parameters, 10-30 depending on how you count.

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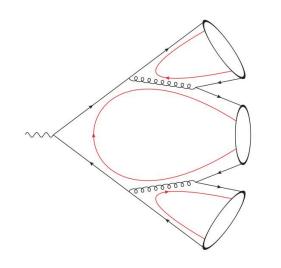
What if we have PS (more perturbative input before hadronization).

The philosophy of the model: use information from perturbative QCD as an input for hadronization. QCD **pre-confinement** discovered by Amati & Veneziano [*Phys.Lett.B* 83 (1979) 87-92]:



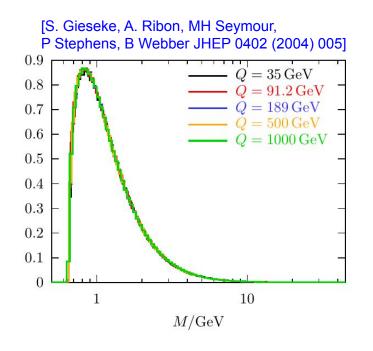
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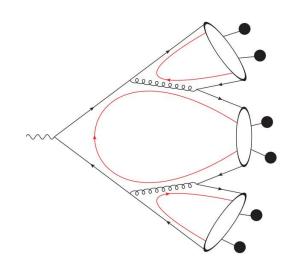
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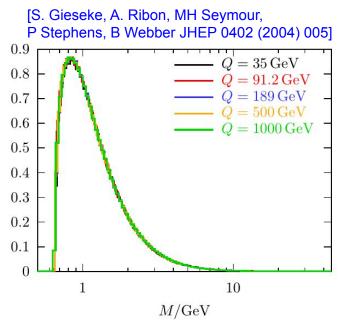
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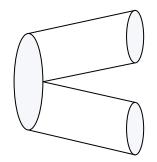


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- Peaked at low mass (1-10 GeV) typically decay into 2 hadrons
- Small fraction of clusters too heavy for isotropic two-body decay, heavy cluster decay first into lighter cluster C → CC, or radiate a hadron C → HC, it is rather string-like.
- ~ 15% of primary clusters get split but ~ 50% of hadrons come from them! (see Simon Pleatzer's talk for some progress)



String vs Cluster model

B^0 B^0 K^+ G^0 C^0 K^+ π^+ π^+ π^+ π^+ π^- π^+ π^-	Jun Received	
program	PYTHIA	Herwig
model	string	cluster
energy–momentum picture	powerful	simple
	predictive	unpredictive
parameters	few	many
flavour composition	messy	simple
	unpredictive	in-between
parameters	many	few

Taken from T. Sjostrand

Colour reconnection in Pythia

Introduced by T. Sjostrand and M. van Zijl [Phys.Rev. D36 (1987) 2019]

to describe SppS data:

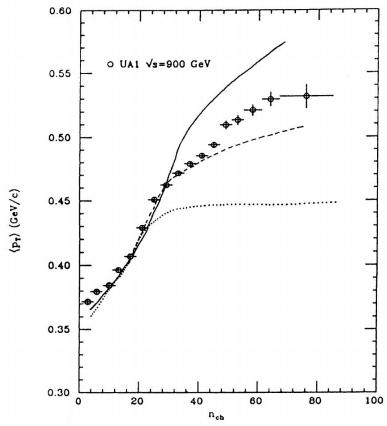
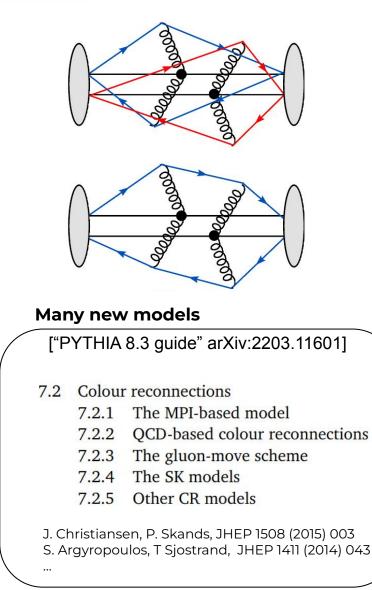


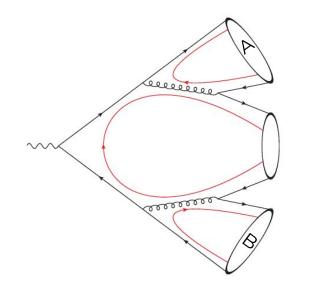
FIG. 27. Average transverse momentum of charged particles in $|\eta| < 2.5$ as a function of the multiplicity. UA1 data points (Ref. 49) at 900 GeV compared with the model for different assumptions about the nature of the subsequent (nonhardest) interactions. Dashed line, assuming $q\bar{q}$ scatterings only; dotted line, gg scatterings with "maximal" string length; solid line gg scatterings with "minimal" string length.

$\langle p_{\perp} angle (n_{ m ch})$ sensitive to colour structure



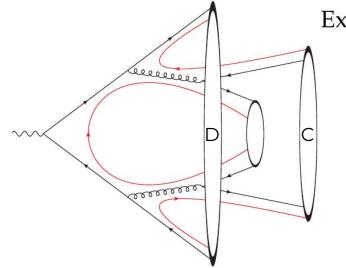
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[Gieseke, Röhr, AS, EPJC 72 (2012)]



Extending Herwig's hadronization model:

 QCD parton showers provide *pre-confinement* ⇒ colour-anticolour pairs form highly excited hadronic states, the *clusters*

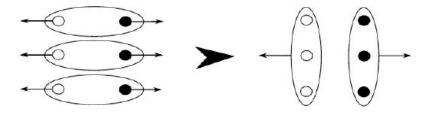


Different approaches in Herwig

Extending Herwig's hadronization model:

- QCD parton showers provide *pre-confinement* ⇒ colour-anticolour pairs form highly excited hadronic states, the *clusters*
 - CR in the cluster hadronization model: allow *reformation* of clusters, if $M_C + M_D < M_A + M_B$ accept alternative clustering with probability p_{reco}

- "Space-time CR" [J. Bellm, C. Duncan, S. Gieseke, M. Myska, AS EPJC 79 (2019) no.12, 1003]
- "Baryonic colour reconnection" [S. Gieseke, P. Kirchgaeßer, S. Plätzer Eur.Phys.J. C78 (2018)]

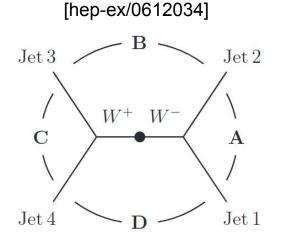


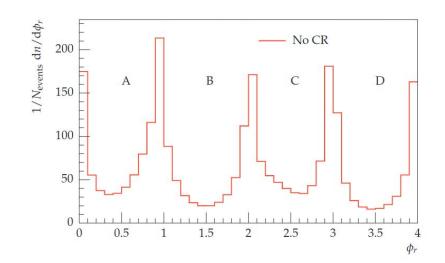
Colour Reconnection from Soft Gluon Evolution [Gieseke, Kirchgaesser, Plätzer, AS JHEP 11 (2018) 149]

(see Simon's Pleatzer talk)

Is Colour reconnection important for lepton colliders?

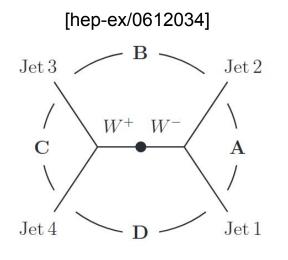
- Effect is less severe than in hadron machines
- However, we are aiming in very precise measurement so we will need to control/constrain it

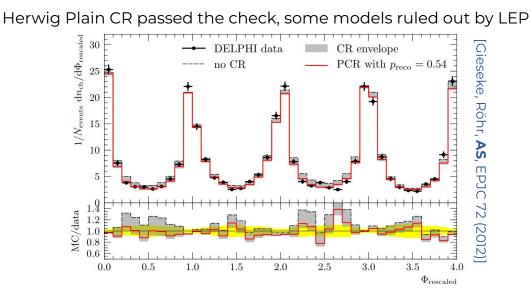




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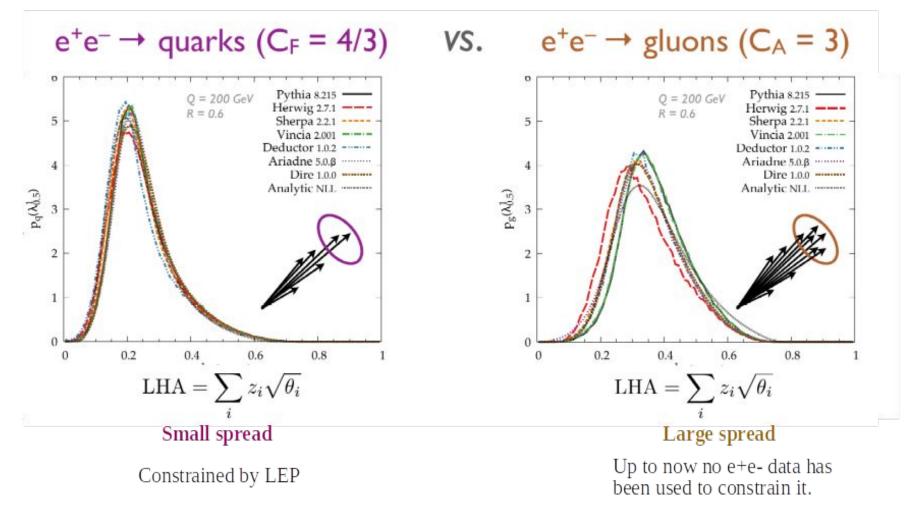
- CR at future e + e colliders [J. Christiansen & T. Sjostrand, EPJ C75 (2015) 9, 441]
 - FCC-ee promises $M_w < 1 \text{ MeV} \Rightarrow$ test CR models by M_w shift in hadronic decays
 - Hadronic Higgs parity measurement ${\rm H}^0 \to {\rm W}^+ {\rm W}^- \to q_1 \overline{q}_2 q_3 \overline{q}_4$ CR important for precision below 5 %
 - Di-photons? (suggested by Stefan Kluth)

Model	$\langle \delta \overline{m}_{ m W} angle$ (MeV)			
would	170 GeV	240 GeV	350 GeV	
SK-I	+18	+95	+72	
SK-II	-14	+29	+18	
SK-II'	-6	+25	+16	
GM-I	-41	-74	-50	
GM-II	+49	+400	+369	
GM-III	+2	+104	+60	
CS	+7	+9	+4	

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Quark/Gluon jets at e+e-

[Gras, Hoeche, Kar, Larkoski, Lönnblad, Plätzer, AS, Skands, Soyez, Thaler, JHEP 1707 (2017) 091]



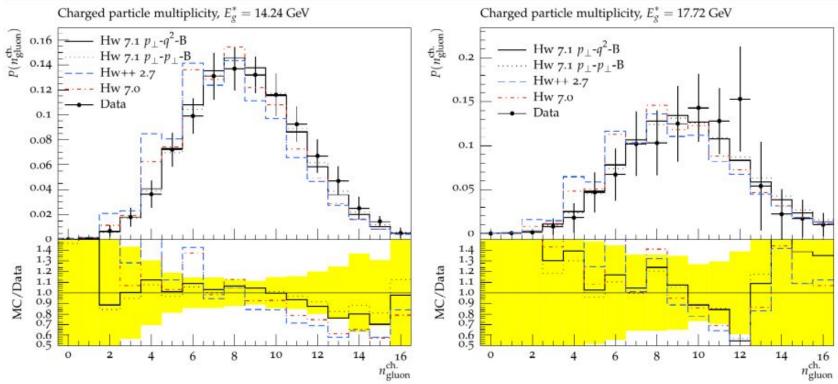
Colour reconnection turned out to be most important here!

Is Colour reconnection important for lepton colliders?

Improving the Simulation of Quark and Gluon Jets with Herwig 7

Daniel Reichelt (Dresden, Tech. U.), Peter Richardson (CERN and Durham U., IPPP), Andrzej Siodmok (Cracow, INP) (Aug 4, 2017) Published in: *Eur.Phys.J.C* 77 (2017) 12, 876 • e-Print: 1708.01491 [hep-ph]

Multiplicity distribution of charged particles in gluons jets for two different gluon energies.

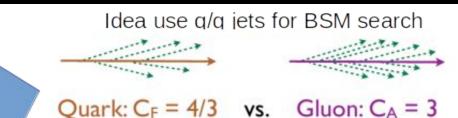


Data was one of the **key for the improvement** and it is still needed for the progress. FCCee will be crucial to constrain the CR and hadronization models.

Similarly like LEP \Rightarrow LHC we will benefit enormously from FCCee \Rightarrow FCChh

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Example of non-perturbative "loop" correction



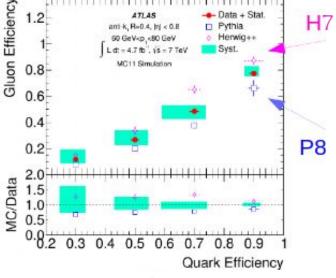






1.2 Data + Stat.

Validate the idea against the data



Improve description of q/g jets in MCEG

[Reichelt, Richardson, Siodmok EPJC C77 (2017)]

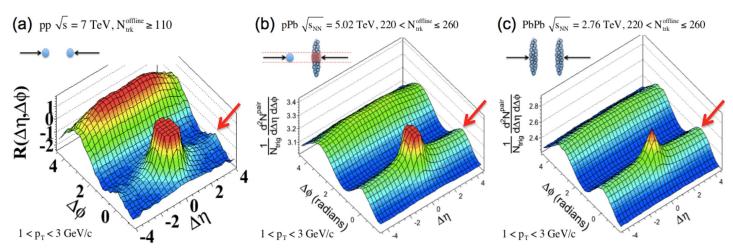


[Gras, Höche, Kar, Larkoski, Lönnblad, Plätzer, Siódmok, Skands, Soyez, Thaler JHEP, 1707, 091 (2017)]

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"A comprehensive guide to the physics and usage of PYTHIA 8.3" [arXiv:2203.11601]

"... hadronization are identical to previous versions of PYTHIA, the past years have seen significant activity in the area of fragmentation dynamics, guided by the discovery of heavy-ion-like effects in hadronic collisions."



Hadronization of very dense systems shows unexpected correlations

LEP 2 data re-analysis shows no correlations in e+e-, worth to measure in FCC-ee!

- 7.3 String interactions and collective effects
 - 7.3.1 String shoving
 - 7.3.2 Rope hadronization
 - 7.3.3 The thermal model

7.3.1 [Ch. Bierlich, S. Chakraborty, G. Gustafson, L. Lönnblad JHEP 03 (2021) 270]
7.3.2 [Ch. Bierlich, S. Chakraborty, G. Gustafson, L. Lönnblad SciPost Phys. 13 (2022)]
7.3.3 [N. Fischer, T. Sjöstrand JHEP 01 (2017) 140]

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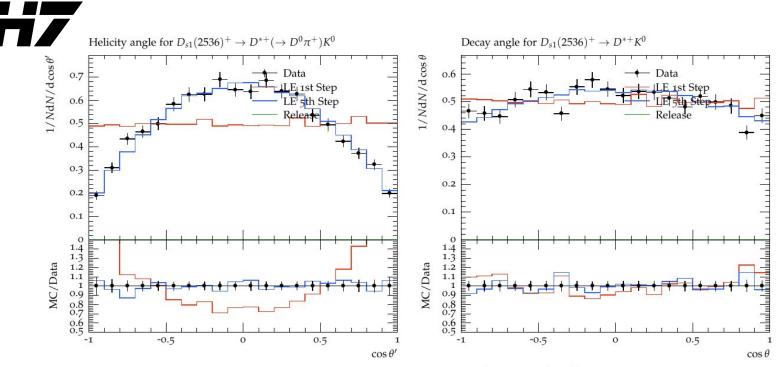
Andrzej Siódmok

 $t = t_3$

 $t = t_A$

 $t = t_2$

Cluster model recent development



LEP measurement of decay angles in the decay $D_{s1}(2536)^+ \rightarrow D^{\star+}K^0$ at $\sqrt{s} = 10.6$ GeV.

- "Polarization of Heavy Hadrons" Aidin Masouminia & Peter Richardson [to be published]
- Dark Cluster Hadronization (see Simon Pleatzer's talk)



Further develop and tune cluster hadronization, and a model for colour reconnection Sherpa (2203.11385).

Tuning

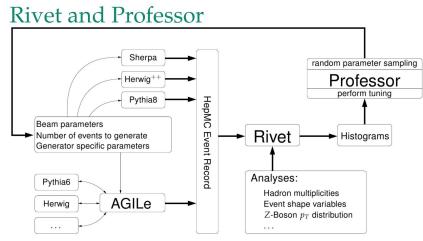
- Fixing parameters of hadronization (tuning) using mainly e+e- LEP data (example next slide)
- A tune encapsulates the knowledge from previous experiments!
- Pythia has plenty tunes, Herwig and Sherpa have much less





Pythia

• Tuning still more like an art than science (many choices to do), however automatized tools: like Professor help a lot!



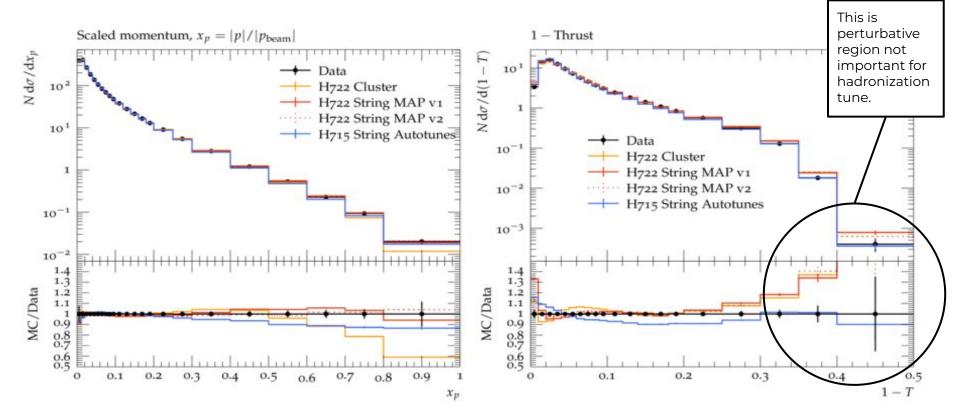
- Warnings:
 - One must be very careful not to overdo tuning (force hadronization to describe perturbative physics - see and S. Pleatzer's talk)
 - Do not ignore past data (some ATLAS tune ignored LEP data, some changes helped to get better description of LHC data but ruined description of LEP)

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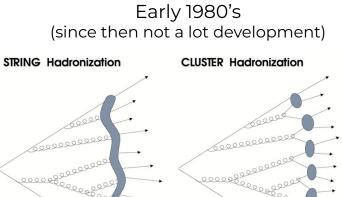
Tuning Angular Ordered PS + String [M.Myska, P. Sarmah, AS to be published]

To **evaluate uncertainties** stemming from the hadronization, Sherpa provides an interface to the Lund string fragmentation in Pythia 6, Herwig has an interface using P8I [Lönnblad] to the Lund string fragmentation in Pythia 8

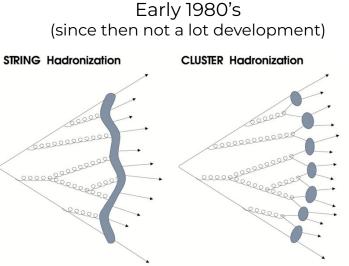
• Plots from the analysis DELPHI_1996_S3430090



Hadronization:



Hadronization:



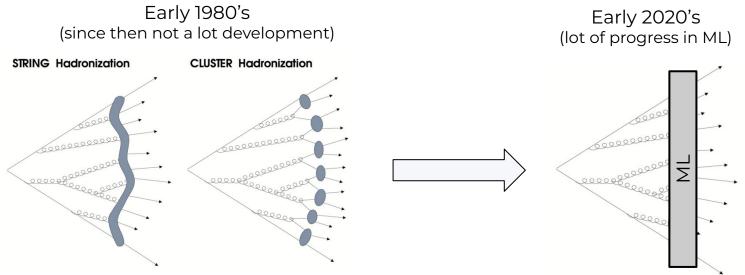
Early 2020's (lot of progress in ML)

	Why keep exploring the energy frontier?
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Exploring the energy frontier is important for several reasons:

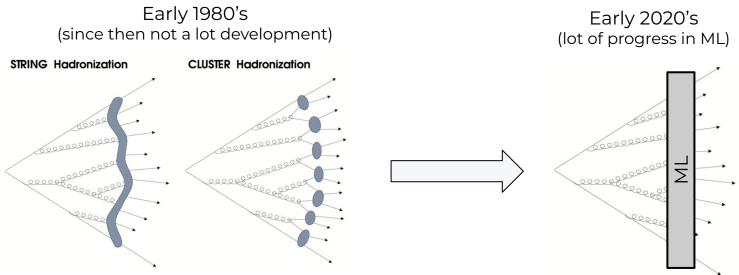
(Gauthier Durieux's talk)

Hadronization:



- → Increased control of perturbative corrections ⇒ more often the precision of LHC measurements is limited by MCEG's non-perturbative components, such as hadronization.
- → Hadronization (phenomenological models with many free parameters ~ 30 parameters)
- → Hadronization is a fitting problem ML is proved to be well suited for such a problems.

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NNPDF

NNPDF used successfully ML to nonperturbative Parton Density Functions (PDF) Early on, lated to fragmentation functions (closely related to hadronization) were considered the counterpart of PDFs.

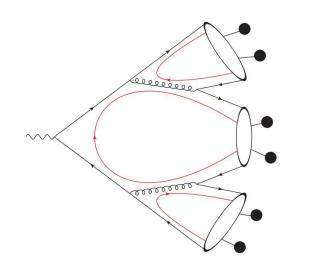
First steps for ML hadronization:

- HADML Generative Adversarial Networks [A. Ghosh, Xi. Ju, B. Nachman **AS**, *Phys.Rev.D* 106 (2022) 9]
- MLhad Variational Autoencoder [P. Ilten, T. Menzo, A. Youssef and J. Zupan, arXiv:2203.04983]

Cluster hadronization model

The philosophy of the model: use information from perturbative QCD as an input for hadronization.

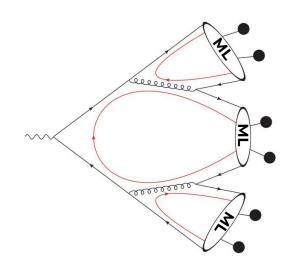
QCD **pre-confinement** discovered by Amati & Veneziano:



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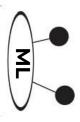
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• ML hadronization

1st step: generate kinematics of a cluster decay:



How?

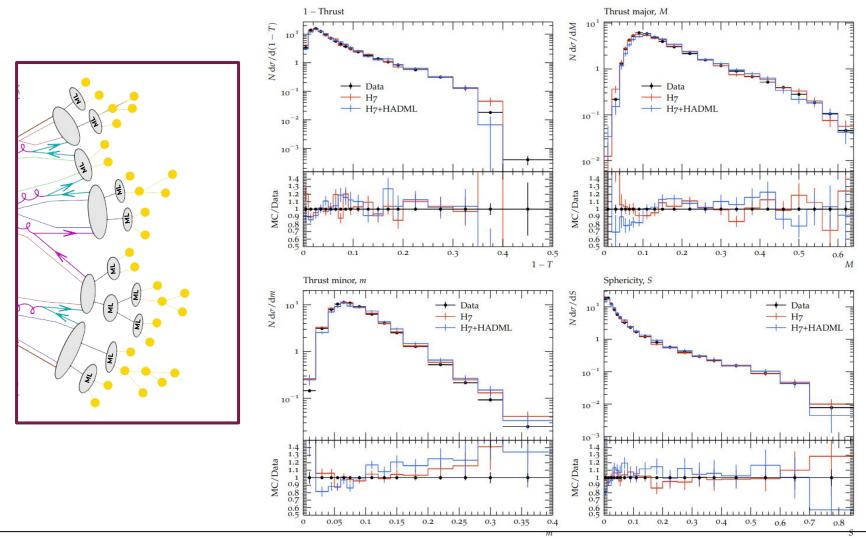
Use Generative Adversarial Networks (GAN)

HADML Results

Full-event Validation

(Full events using HADML integrated into Herwig 7)

LEP DELPHI Data



The ultimate goal of is to train the ML model directly on data to improve hadronization models.

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Summary and Outlook

- Progress in perturbative QCD ⇒ more often measurements are limited by hadronization.
- Two different models of hadronization: string and clasters (early 80's)
 + some new elements (collective effects, polarization, ...)
- Both have weak and strong sides useful for systematics.
- A tune encapsulates the knowledge from previous experiments!
- Colour reconnection it is important to constrain it.
- Better Hadronization
 - Steady improvements of string and cluster models.
 - New measurements.
 - Better control of the interface of PS and hadronization.
 - Lattice QCD?
 - Machine Learning?



postdoc in ML/HEP positions openings





If you are interested please contact me: andrzej@cern.ch

Minimax Loss

In the paper that introduced GANs, the generator tries to minimize the following function while the discriminator tries to maximize it:

$$E_x[log(D(x))] + E_z[log(1 - D(G(z)))]$$

In this function:

- D(x) is the discriminator's estimate of the probability that real data instance x is real.
- Ex is the expected value over all real data instances.
- G(z) is the generator's output when given noise z.
- D(G(z)) is the discriminator's estimate of the probability that a fake instance is real.
- E_z is the expected value over all random inputs to the generator (in effect, the expected value over all generated fake instances G(z)).
- The formula derives from the cross-entropy between the real and generated distributions.

The generator can't directly affect the log(D(x)) term in the function, so, for the generator, minimizing the loss is equivalent to minimizing log(1 - D(G(z))).

AlphaGo

- AlphaGo's victory against Lee Sedol was a major milestone in artificial intelligence research.
- Go had previously been regarded as a hard problem in machine learning that was expected to be out of reach for the technology of the time.
- Most experts thought a Go program as powerful as AlphaGo was at least five years away;some experts thought that it would take at least another decade before computers would beat Go champions. Most observers at the beginning of the 2016 matches expected Lee to beat AlphaGo.
- Netflix document

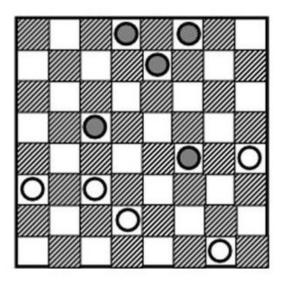


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Adversarial Networks

Arthur Lee Samuel (1959) wrote a program that learnt to play checkers well enough to beat him.





- He popularized the term "machine learning" in 1959.
- The program chose its move based on a **minimax** strategy, meaning it made the move assuming that the opponent was trying to optimize the value of the same function from its point of view.
- He also had it play thousands of **games against itself** as another way of learning.

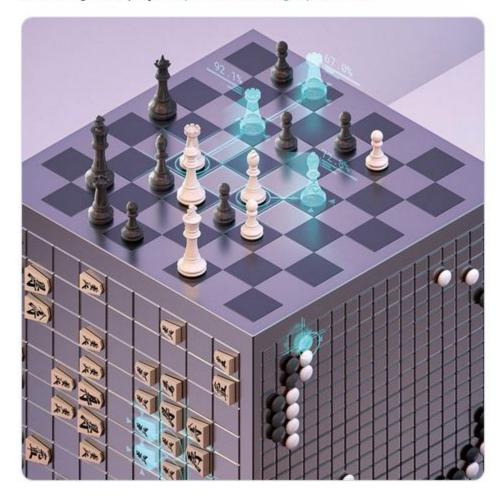
Adversarial Networks



DeepMind 🤣 @DeepMind · Dec 6, 2018



The full peer-reviewed @sciencemagazine evaluation of #AlphaZero is here - a single algorithm that creatively masters chess, shogi and Go through self-play deepmind.com/blog/alphazero...





By playing games against itself, AlphaGo Zero surpassed the strength of <u>AlphaGo Lee</u> in three days by winning 100 games to 0.

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Adversarial Networks

tl You Retweeted



OpenAl 🤣 @OpenAl

We trained a neural network that solved two problems from the International Math Olympiad. openai.com/blog/formal-ma...

```
theorem imo_longlist_1990_p77
  (a * b + b * c + c * a)^3 ≤
      (a^2 + a * b + b^2) * (b^2 + b * c + c^2) *
      (c^2 + c * a + a^2)
begin
   let u : euclidean_space ℝ (fin 2) := ![a, b],
   let v : euclidean_space ℝ (fin 2) := ![b, c],
   have h₀ := real_inner_mul_inner_self_le u v,
   ...
```



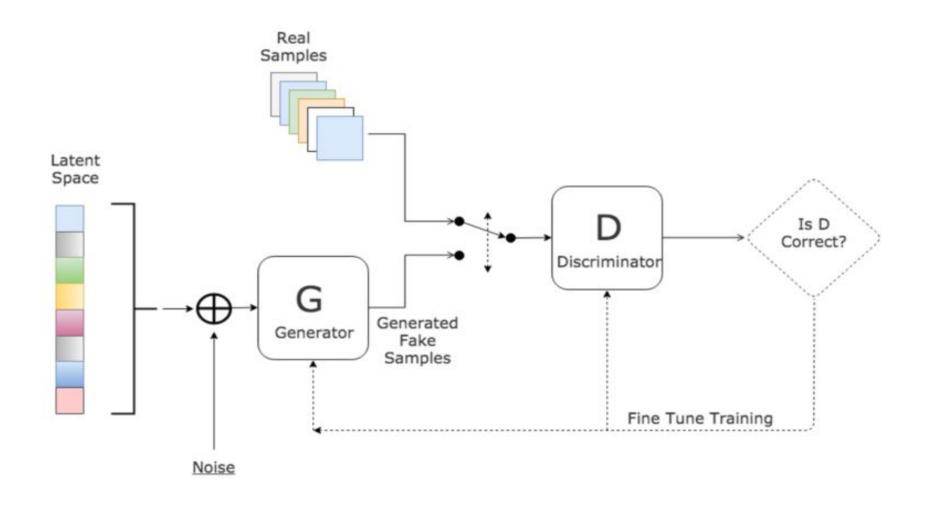


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99 Retweets 32 Quote Tweets 564 Likes

Generative Adversarial Network (GAN)

[Goodfellow et al. "Generative adversarial nets". arxiv:1406.2661]



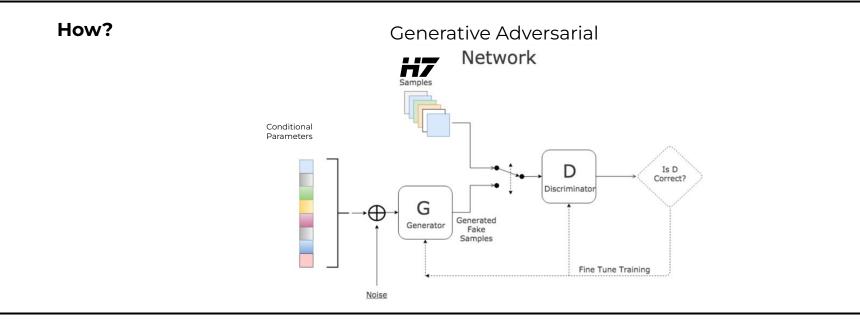
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Towards a Deep Learning Model for Hadronization

ML hadronization

1st step: generate kinematics of a cluster decay to 2 hadrons





Training data:

 e^+e^- collisions at $\sqrt{s} = 91.2 \text{ GeV}$

Cluster
$$(E, p_x, p_y, p_z)$$

$$\pi^{0}(E, p_x, p_y, p_z)$$

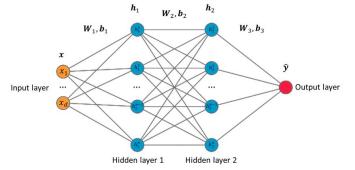
Pert = 0/1 memory of quarks direction

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Architecture: conditional GAN

Generator and the Discriminator are composed of two-layer perceptron

(each a fully connected, hidden size 256, a batch normalization layer, LeakyReLU activation function)



Generator

Input

Cluster (E, p_x, p_y, p_z) and 10 noise features sampled from a Gaussian distribution

Output (in the cluster frame)

$$\left. \begin{array}{l} \phi & - \text{ polar angle} \\ \theta & - \text{ azimuthal angle} \end{array} \right\}$$

we reconstruct the four vectors of the two outgoing hadrons

Discriminator

Input

 ϕ and heta labeled as signal (generated by Herwig) or background (generated by Generator)

Output

Score that is higher for events from Herwig and lower for events from the Generator

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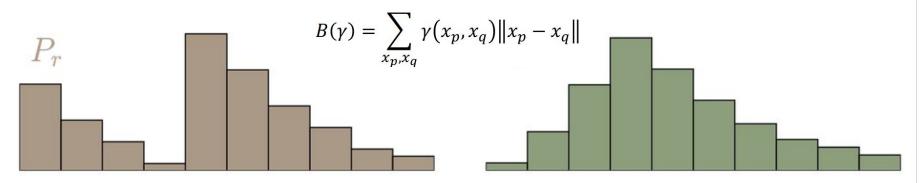
Wasserstein distance

The Wasserstein distance

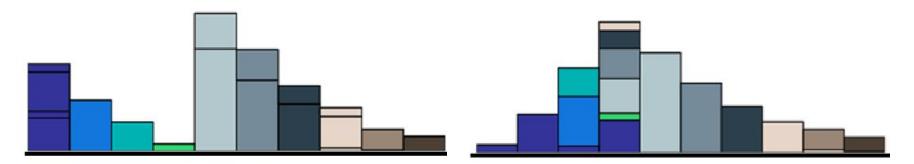
- For discrete probability distributions, the Wasserstein distance is called the earth mover's distance (EMD):
- EMD is the minimal total amount of work it takes to transform one heap into the other.

$$W(P,Q) = \min_{\gamma \in \Pi} B(\gamma)$$

• Work is defined as the amount of earth in a chunk times the distance it was moved.



Best "moving plans" of this example



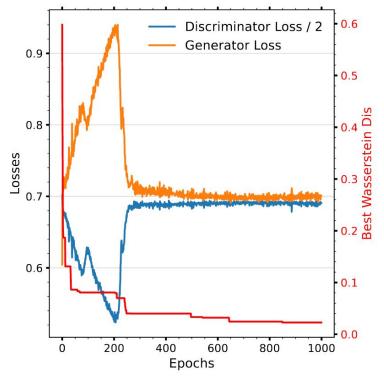
5th Inter-experiment Machine Learning Workshop

Training

• Data normalization:

cluster's four vector and angular variables are scaled to be between -1 and 1 (tanh activation function as the last layer of the Generator)

• **Discriminator** and the **Generator** are trained separately and alternately by two independent Adam optimizers with a learning rate of 10⁻⁴, for 1000 epochs



• **The best model** for events with partons of Pert = 0, is found at the epoch 849 with a total Wasserstein distance of 0.0228.

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Investigation of Colour Reconnection in WW events with the DELPHI detector at LEP-2

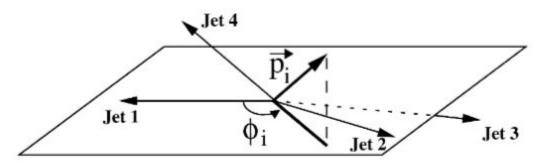


Fig. 1. Determination of the ϕ_i angle for the particle *i*.

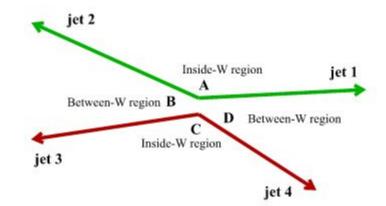
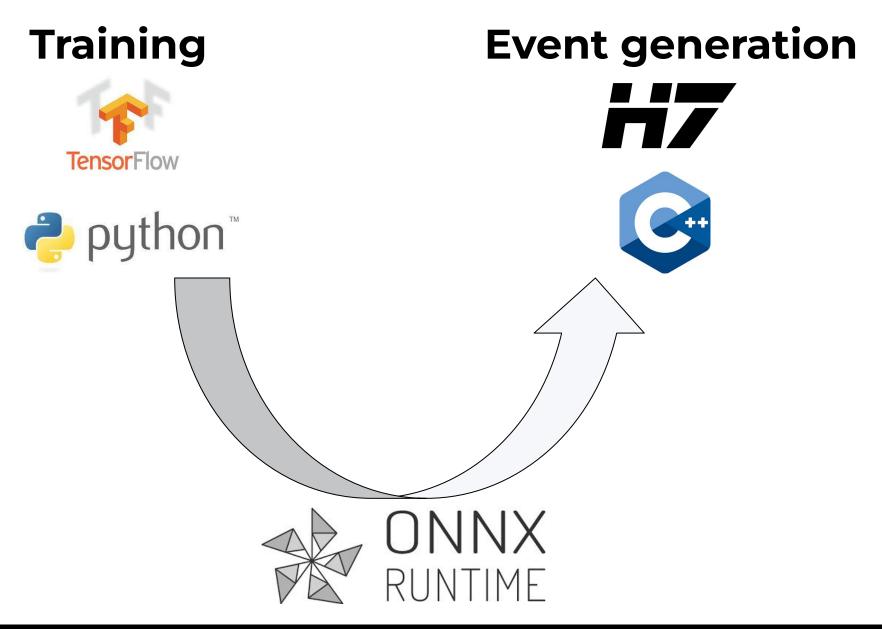


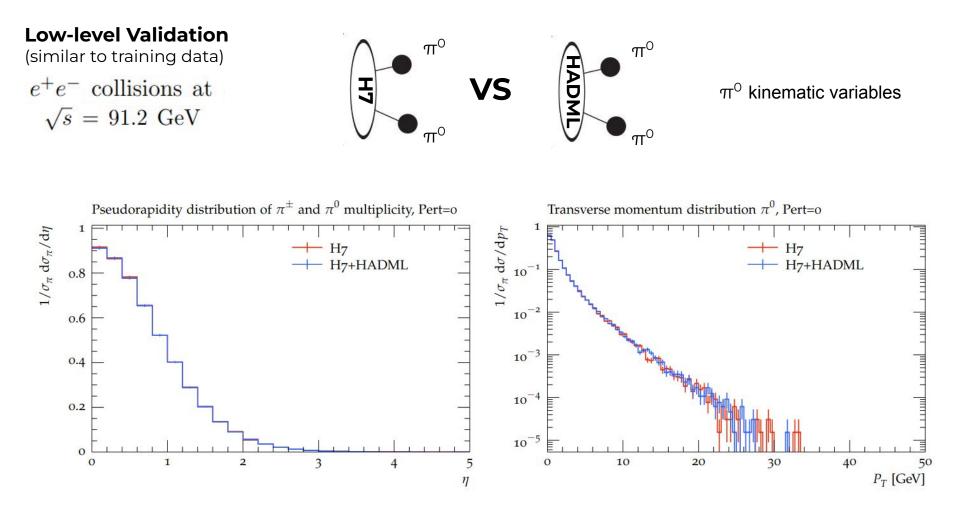
Fig. 3. Schematic drawing of the angular selection

In order to compare the interjet regions the angles in the planes are rescaled by the angle between the two closest jets. For a particle *i* located between jets *j* and j + 1 the rescaled angle is

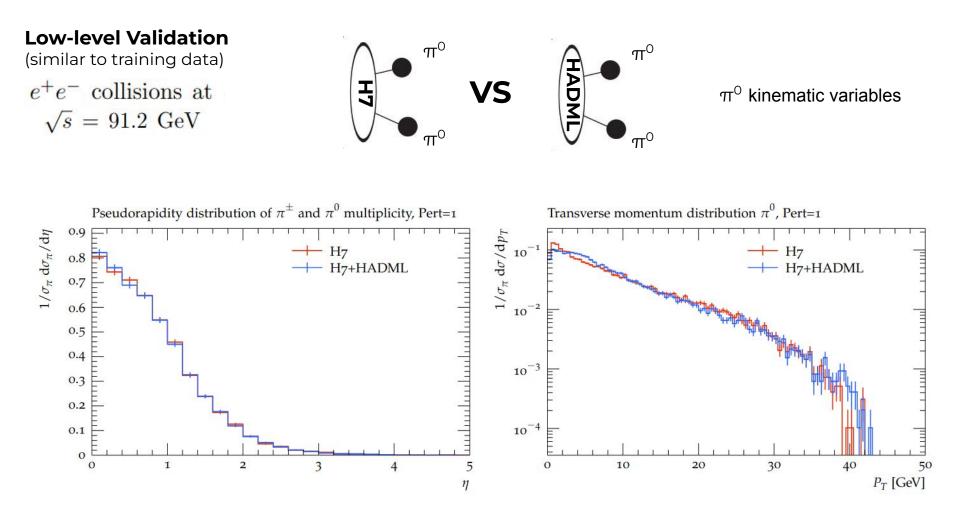
$$\phi_i^{\text{resc}} = j - 1 + \frac{\phi_{j,i}}{\psi_{j,j+1}},$$
(2)

Integration into Herwig

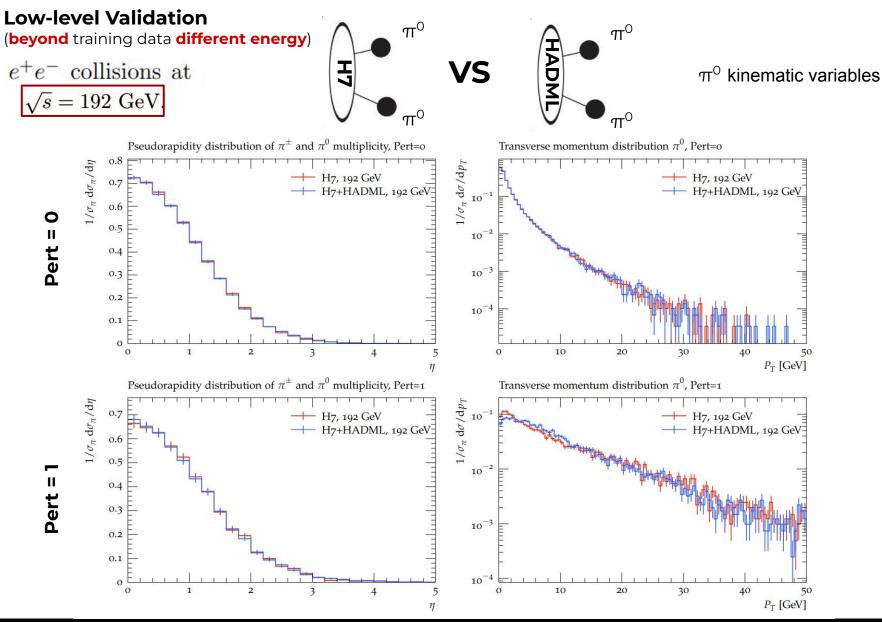




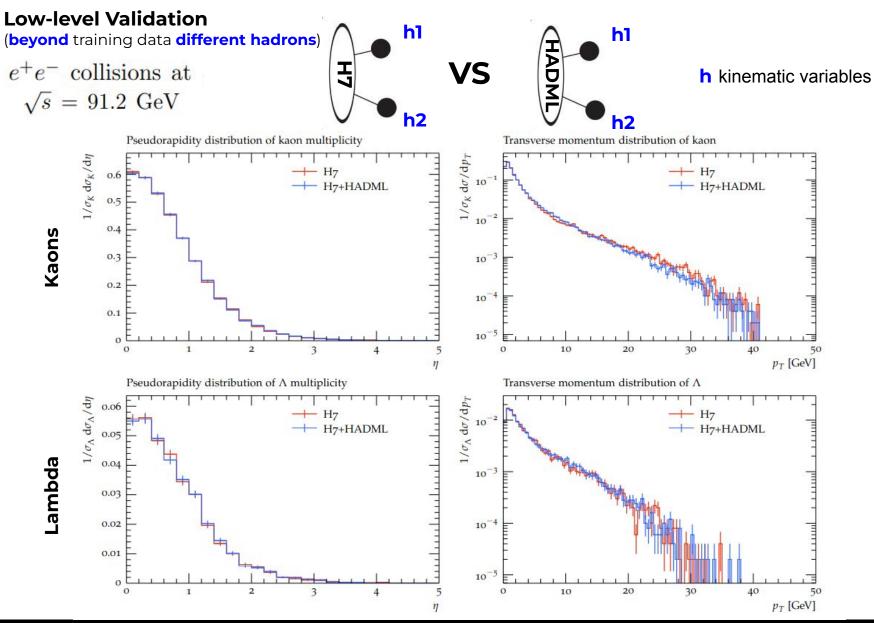
Pert = 0 (no memory of quark kinematics)



Pert = 1 (memory of quark kinematics)

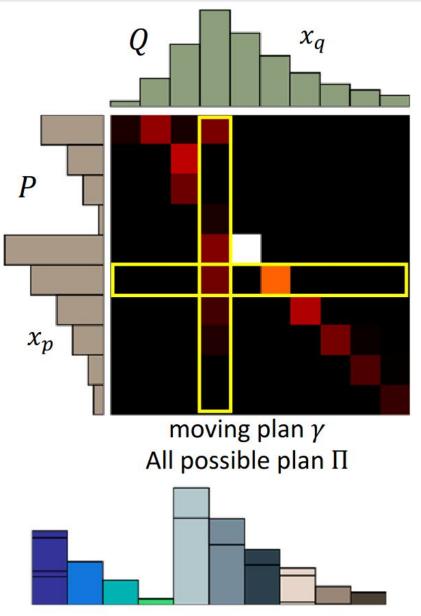


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Wasserstein distance



A "moving plan" is a matrix The value of the element is the amount of earth from one position to another.

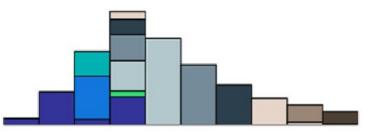
Average distance of a plan γ :

$$B(\gamma) = \sum_{x_p, x_q} \gamma(x_p, x_q) \|x_p - x_q\|$$

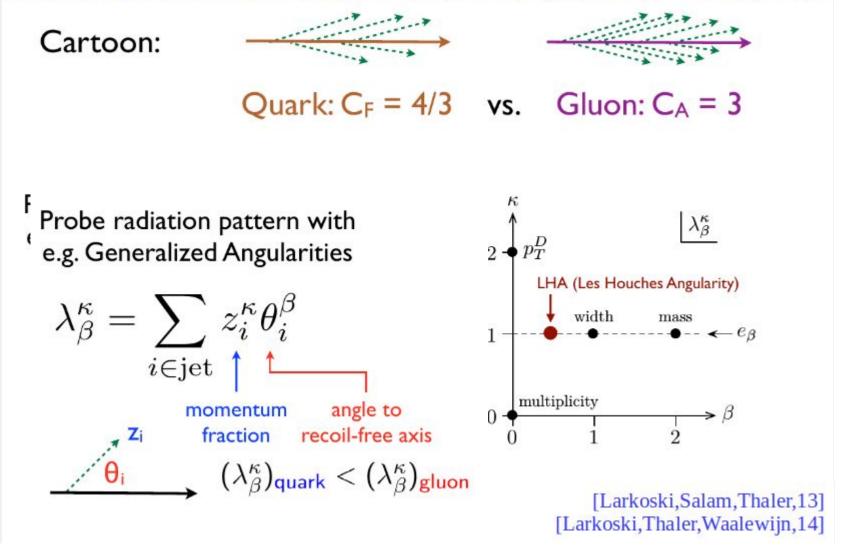
Earth Mover's Distance:

$$W(P,Q) = \min_{\gamma \in \Pi} B(\gamma)$$

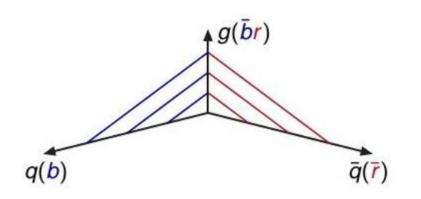
The best plan





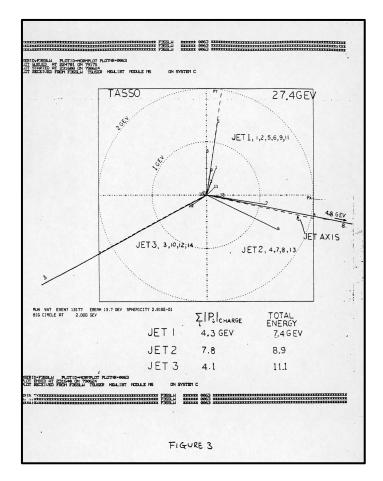


Gluons - a kink in the string



The Lund string model predicted the string effect measured by Jade.

In a three-jet event there are more energy between the gq and gq jets than between qq.



Summary:

String model has very good energy-momentum picture however it is unpredictive in understanding of hadron mass effects \Rightarrow many parameters, 10-30 depending on how you count.

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Polarization of Heavy Hadrons

1st Step: Passing through the polarization of heavy hadrons at the end of parton shower. [arXiv:hep-ph/9308241]

- For $m_Q \gg \Lambda_{\rm QCD}$, the light degrees of freedom become insensitive to m_Q .
- Heavy quarks act as non-recoiling sources of color at the end of PS.
- A spin-flavor symmetry appears for heavy quarks.
- A net polarization of the initial heavy quark may be detected, either in a polarization of the final ground state or in the decay products of the excited heavy mesons and heavy baryons.
- Falk-Peskin "no-win" theorem: no polarization information would be found in non-excited mesons.

2nd Step: Improving the Strong decay modes the excited heavy mesons, i.e charm, and bottom mesons.

- Heavy Quark Effective Field Theory (HQEFT) usually determines which decay modes are possible and also gives the relations between the involving couplings.
- In the absence of experimental data on many of the decays, we need to rely on HQ symmetries to determine the decay modes, widths and branching ratios.
- We consider charm and bottom meson decays with:

[arXiv:hep-ph/9209239]

•
$$J^P = 0^-, 1^-$$
 doublets with $l = 0$ (D and D^{*}).

- $J^P = 1^+, 2^+$ doublets with l = 1 and j = 3/2 (D_1 and D_2^*).
- $\circ J^P = 0^+, 1^+$ doublets with l = 1 and j = 1/2 (D_0^* and D_1').

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