Department of Theoretical Physics

A path to accurate and physical event generators with PanScales

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Würzburg Seminar Teilchentheorie

Based on
Phys.Rev.Lett. 131 (2023) 16 [Ferrario Ravasio, Hamilton, AK, Salam, L. Scyboz, G. Soyez]
Phys.Rev.Lett. 134 (2025) 01 [eid. + M. v. Beekveld, M. Dasgupta, B. K. El-Menoufi, J. Helliwell, P. F. Monni, A. Soto-Ontoso]

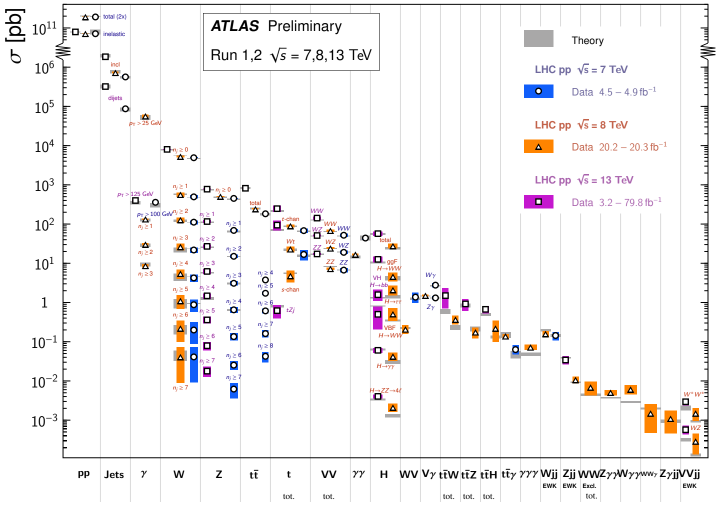
+

2504.05377 with M. v. Beekveld, S. Ferrario Ravasio, J. Helliwell, G. Salam, L. Scyboz, A. Soto-Ontoso, G. Soyez, and S. Zanoli

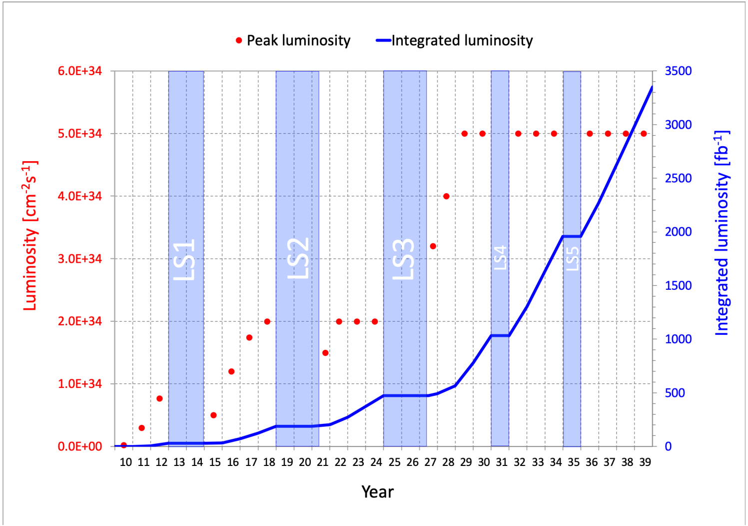
The precision era of the LHC

Standard Model Production Cross Section Measurements

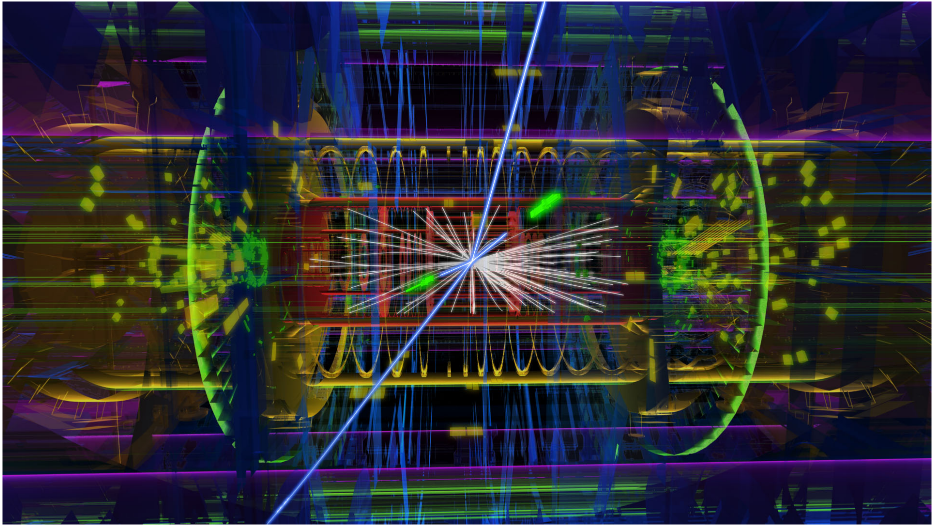
Status: July 2018



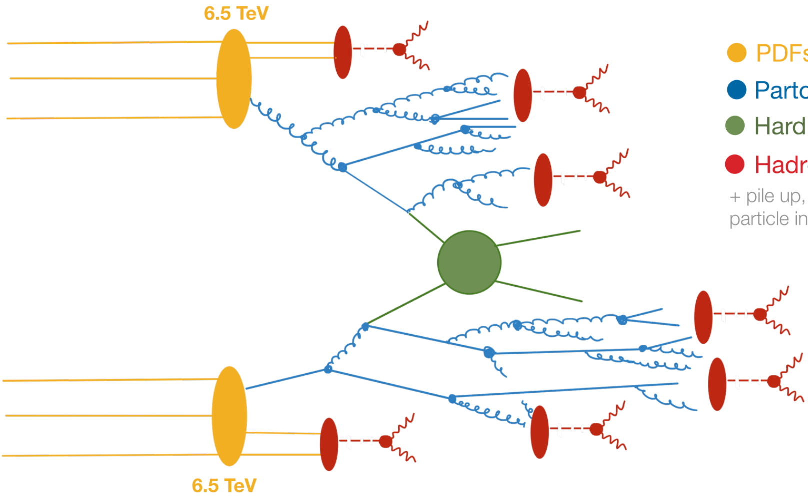
The precision era of the LHC



The LHC: A messy environment



Anatomy of an LHC collision



- PDFs / beam remnants
- Parton shower $\mathcal{O}(1-100)$ **GeV**
- Hard scattering $\mathcal{O}(0.1-1)$ **TeV**
- Hadronisation $\mathcal{O}(1)$ **GeV**

+ pile up, underlying event, multiple-particle interactions (MPI)…

courtesy M. van Beekveld

The ubiquitous Parton Shower

Pythia 8

An introduction to PYTHIA 8.2 #1

Torbjörn Sjöstrand (Lund U., Dept. Theor. Phys.), Stefan Ask (Cambridge U.), Jesper R. Christiansen (Lund U., Dept. Theor. Phys.), Richard Corke (Lund U., Dept. Theor. Phys.), Nishita Desai (U. Heidelberg, ITP) et al. (Oct 11, 2014)

Published in: *Comput.Phys.Commun.* 191 (2015) 159-177 • e-Print: 1410.3012 [hep-ph]

pdf links DOI cite 6,423 citations

Herwig 7

Herwig++ Physics and Manual #1

M. Bahr (Karlsruhe U., ITP), S. Gieseke (Karlsruhe U., ITP), M.A. Gigg (Durham U., IPPP), D. Grellscheid (Durham U., IPPP), K. Hamilton (Louvain U.) et al. (Mar, 2008)

Published in: *Eur.Phys.J.C* 58 (2008) 639-707 • e-Print: 0803.0883 [hep-ph]

pdf links DOI cite 3,150 citations

Sherpa

Event generation with SHERPA 1.1 #1

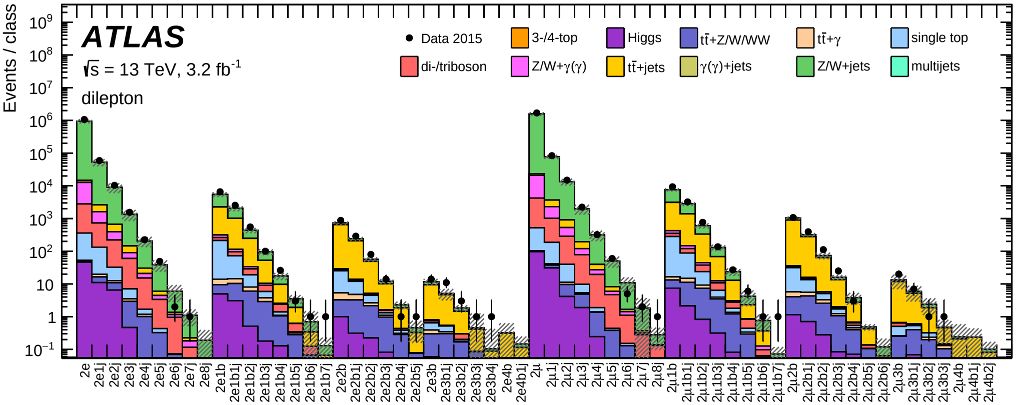
T. Gleisberg (SLAC), Stefan. Hoeche (Zurich U.), F. Krauss (Durham U., IPPP), M. Schonherr (Dresden, Tech. U.), S. Schumann (Edinburgh U.) et al. (Nov, 2008)

Published in: *JHEP* 02 (2009) 007 • e-Print: 0811.4622 [hep-ph]

pdf links DOI cite 3,827 citations

Parton Showers enter one way or another in almost 95% of all ATLAS and CMS analyses. Collider physics would not be the same without them.

The ubiquitous Parton Shower



ATLAS [1807.07447]

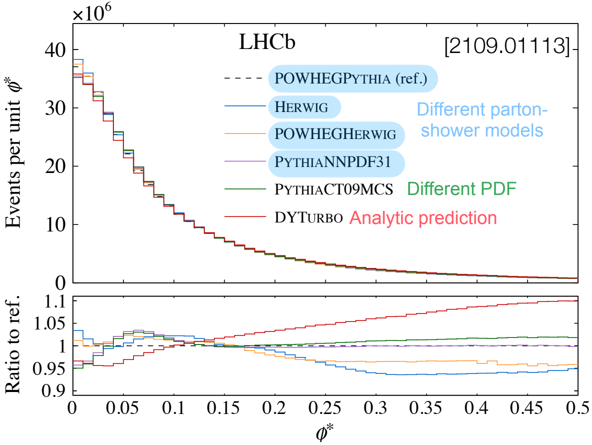
But differences matter…

Consider measurement of W boson mass

Measurements of p_T^Z in $Z/\gamma^* \to l^+l^-$ decays used to validate the MC predictions for p_T^W

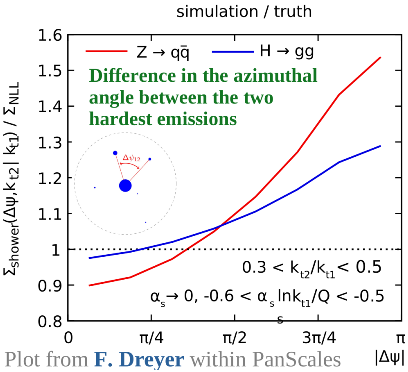
The envelope of shifts in m_W originating from differences in these shower predictions is the dominant theory uncertainty (11 MeV)

$$m_W = 80354 \pm 23_{\text{stat}} \pm 10_{\text{exp}} \pm 17_{\text{theory}} \pm 9_{\text{PDF}}\ \text{MeV}$$

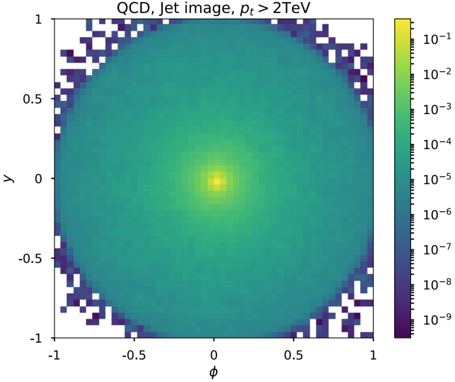


$$\phi^* = \frac{\tan((\pi - \Delta\phi)/2)}{\cosh(\Delta\eta/2)} \sim \frac{p_T^Z}{m_{ll}}$$ [1009.1580]

Machine learning and jet sub-structure

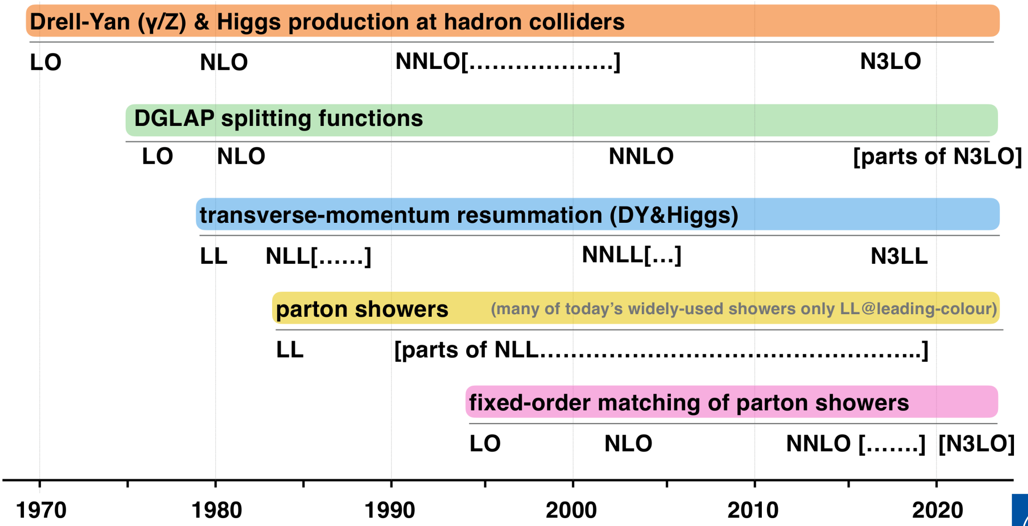


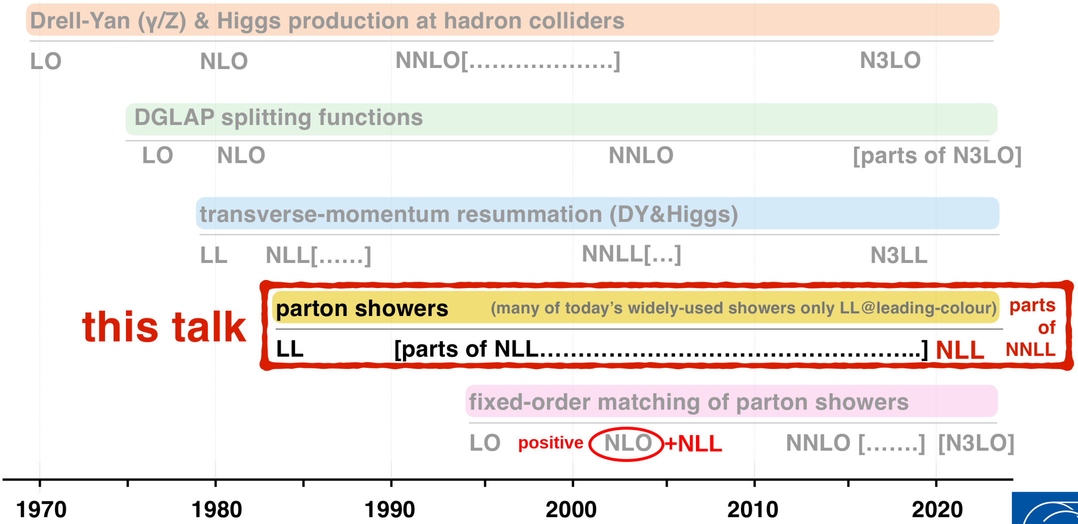
Plot from **F. Dreyer** within PanScales



de Oliveira, Kagan, Mackey, Nachmann, Schwartzman [1511.05190]

Machine learning might learn un-physical "features" from MC $\rightarrow$ can significantly impact the potential of new physics searches.


Drell-Yan (γ/Z) & Higgs production at hadron colliders
LO
NLO
NNLO[..................]
N3LO
DGLAP splitting functions
LO
NLO
NNLO
[parts of N3LO]
transverse-momentum resummation (DY&Higgs)
LL
NLL[......]
NNLL[...]
N3LL
parton showers
(many of today's widely-used showers only LL@leading-colour)
LL
[parts of NLL..]
fixed-order matching of parton showers
LO
NLO
NNLO [.......]
[N3LO]
1970
1980
1990
2000
2010
2020


Drell-Yan (γ/Z) & Higgs production at hadron colliders
LO
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transverse-momentum resummation (DY&Higgs)
LL
NLL[......]
NNLL[...]
N3LL
this talk
parton showers
(many of today's widely-used showers only LL@leading-colour)
parts of NNLL
LL
[parts of NLL...]
NLL
fixed-order matching of parton showers
LO
positive
NLO
+NLL
NNLO [.......]
[N3LO]
1970
1980
1990
2000
2010
2020

Why are we talking about logarithmic accuracy?

Parton showers evolve hard states $Q \sim \sqrt{\hat{s}}$ down to the scale where hadronisation takes place $\Lambda \sim 1$ GeV

This evolution generates logarithms of the form $L \sim \ln\frac{Q}{\Lambda} \gg 1$, $(g_X(\alpha_s L) \sim \alpha_s L)$

$$\Sigma(\mathcal{O} < e^{-L}) = \exp\Big[-L g_{LL}(\alpha_s L) + g_{NLL}(\alpha_s L) + \alpha_s g_{NNLL}(\alpha_s L) + \ldots\Big]$$

	$Q = M_Z$	$Q = 1$ TeV	
$\lvert L g_{LL}\rvert \sim \alpha_s L^2$	2	4	
$\lvert g_{NLL}\rvert \sim \alpha_s L$	0.5	0.6	$\leftarrow \mathcal{O}(100\%)$
$\lvert \alpha_s g_{NNLL}\rvert \sim \alpha_s^2 L$	0.06	0.05	$\leftarrow \mathcal{O}(10\%)$

NNLL crucial to reach percent-level accuracy!

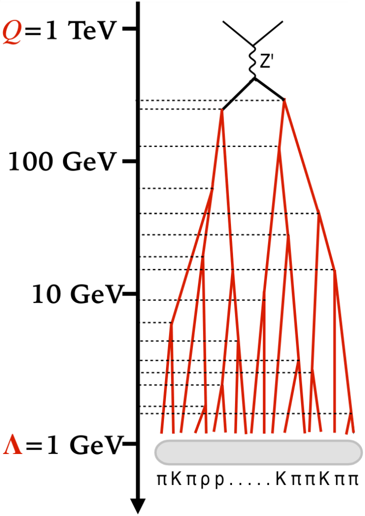


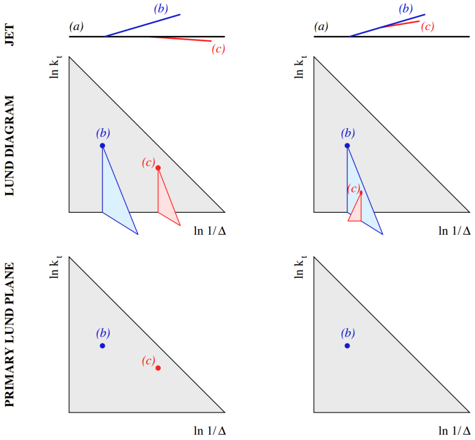
Figure by S. Ferrario Ravasio

Current status of parton showers

- The most widely-used event generators at the LHC, Pythia, Herwig, and Sherpa, are all limited to LL (some exceptions where NLL can be reached, cf. Bewick, Ferrario Ravasio, Richardson, Seymour [1904.11866])
- Although there has been significant progress in improving the hard matrix elements of event generators with NNLO matching and NLO multi-jet merging, the logarithmic accuracy has been limited to LL for a very long time
- For this reason, there has been a concerted effort in taking parton showers from LL→NLL in the last couple of years
- This has been achieved by several groups including PanScales [1805.09327], [2002.11114], [2011.10054], [2103.16526], [2111.01161], [2205.02237], [2207.09467], [2305.08645], [2312.13275], [2406.02661], ALARIC Herren, Höche, Krauss, Reichelt, Schoenherr [2208.06057], [2404.14360], APOLLO Preuss [2403.19452], DEDUCTOR Nagy, Soper [2011.04773], and Forshaw-Holguin-Plätzer [2003.06400]

→ Very recently we have taken significant steps towards general NNLL (focus of this talk)

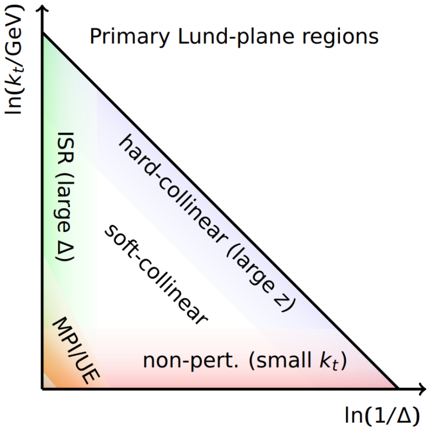
The Lund Plane



Dreyer, Salam, Soyez [1807.04758]

- To better make the connections between parton showers and their logarithmic accuracy we need to introduce the Lund Plane:
- Cluster the event with the Cambridge/Aachen algorithm, producing an angular ordered clustering sequence.
- Decluster the last clustering and record the transverse momentum and the opening angle of the declustering (plus other kinematics).
- Iterate along the hardest branch after each declustering to produce the primary Lund Plane.
- Following the softer branch produces the secondary, tertiary, etc Lund Plane.
- One can impose cuts easily on the declusterings (e.g. that they satisfy $z > z_{\mathrm{cut}}$)

Logarithms in the Lund Plane

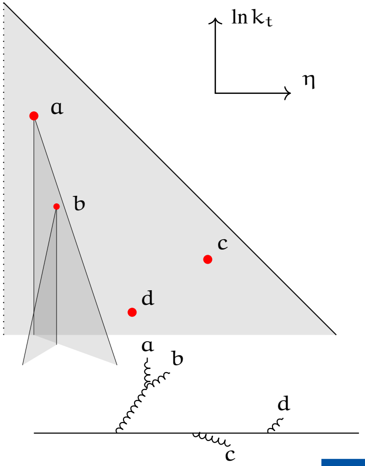


Dreyer, Salam, Soyez [1807.04758]

- The emission probability in the Lund Plane is then
$$d\rho \sim \alpha_s \, d\ln k_T \, d\ln\theta$$
- Hence emissions that are well-separated in both directions are associated with double logarithms of the form $\alpha_s^n L^{2n}$
- Emissions separated along one direction are associated with single logarithms of the form $\alpha_s^n L^n$
- Emissions that are close in the Lund Plane are associated with a factor α_s^n
- We are now ready to state the PanScales NLL criteria for Parton Showers

NLL showers in a nutshell

- A necessary condition for a shower to be NLL is that it correctly describes configurations where all emissions are well-separated in a Lund plane Dasgupta, Dreyer, Hamilton, Monni, Salam [1805.09327]
- A core principle in this picture is that two emissions that are well-separated, should not influence each other (e.g. emission d cannot change the kinematics of c).[a]
- This principle is violated by most standard dipole-showers, due to the way the recoil is distributed after an emission First observed by Andersson, Gustafson, Sjogren '92
- For NLL 2-loop running coupling in the CMW scheme is also required
- For full NLL one also needs to include spin-correlations and sub-leading colour corrections



[a] Spin-correlations are an exception in this context as they introduce long-range azimuthal correlations at NLL. Collinear spin understood in angular ordered showers for decades due to work of Collins '88 and Knowles '88. Extension to dipole showers studied in Richardson, Webster [1807.01955]. Both collinear and soft spin-correlations are included in PanScales at NLL.

PanLocal

$k_t\sqrt{\theta}$ ordered

Recoil

$\perp$: local

$+$: local

$-$: local

Dipole partition

event CoM

PanGlobal

k_t or $k_t\sqrt{\theta}$ ordered

Recoil

$\perp$: global

$+$: local

$-$: local

Dipole partition

event CoM

e^+e^-: Dasgupta, Dreyer, Hamilton, Monni, Salam, Soyez [2002.11114]; pp (w/spin+colour): van Beekveld, Ferrario Ravasio, Salam, Soto-Ontoso, Soyez, Verheyen [2205.02237]; + pp tests: eid. + Hamilton [2207.09467]; DIS+VBF: van Beekveld, Ferrario Ravasio [2305.08645]

Colour

nested ordered double soft (NODS)

Designed to ensure LL are full colour (also gets many NLL at full colour)

Hamilton, Medves, Salam, Scyboz, Soyez [2011.10054]

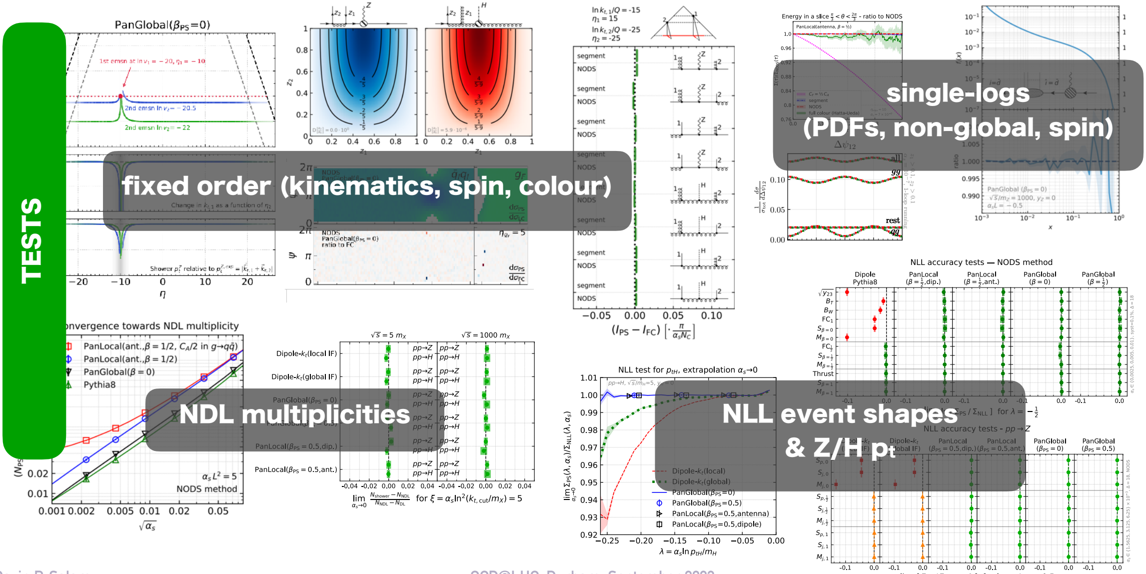
Spin

for correct azimuthal structure in collinear and soft→collinear

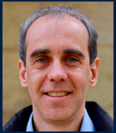
[Collins-Knowles extended to soft sector]

AK, Salam, Scyboz, Verheyen [2103.16526], eid. + Hamilton [2111.01161]

a selection of the logarithmic accuracy tests



Oxford



Gavin Salam

Nicolas Schalch

Silvia Zanoli

Monash

Ludovic Scyboz

Basem El-Menoufi

Jack Helliwell

CERN

AK

Pier Monni

Silvia Ferrario Ravasio

UCL

Keith Hamilton

Manchester

Mrinal Dasgupta

NIKHEF

Melissa van Beekveld

IPhT

Gregory Soyez

UGR

Alba Soto-Ontoso

PanScales current members

A project to bring logarithmic understanding and accuracy to parton showers

Analytic structure beyond NLL

Taking an event shape, $\mathcal{O}$, to be less than some value $e^{-|L|}$ we have at NNLL (focusing for now on e^+e^- only)

$$\Sigma(\mathcal{O} < e^{-|L|}) = (1 + \alpha_s C_1 + \dots) \exp\left[\frac{1}{\alpha_s} g_1(\alpha_s L) + g_2(\alpha_s L) + \alpha_s g_3(\alpha_s L) + \dots\right] \quad (1)$$

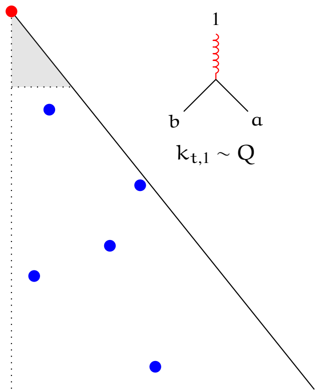
where g_1 accounts for LL terms, g_2 for NLL terms, and g_3 and C_1 for NNLL terms[1]. Whereas an analytic resummation in principle retains only the terms that are put in (i.e. g_1 and g_2 at NLL) the shower will instead generate spurious higher order terms

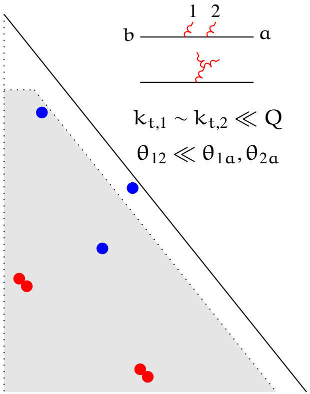
$$\Sigma(\mathcal{O} < e^{-|L|}) = \left(1 + \alpha_s \tilde{C}_1 + \dots\right) \exp\left[\frac{1}{\alpha_s} g_1(\alpha_s L) + g_2(\alpha_s L) + \alpha_s \tilde{g}_3(\alpha_s L) + \dots\right] \quad (2)$$

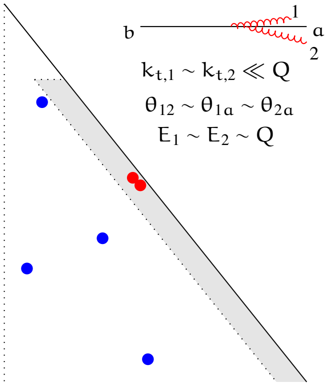
When thinking about going beyond NLL we need to address two things: 1) what are the necessary analytic ingredients from resummation and 2) how do we compensate the NNLL terms already present in the shower?

[1]In the language of q_T resummation A_1 is responsible for LL terms, A_2 and B_1 for NLL terms and A_3 and B_2 for NNLL terms (together with the hard coefficient function $C_1(z)$).

Lund plane picture







hard matching →
α_s correct for first emission

double-soft →
get any pair of soft commen--surate energy/angle right

triple-collinear →
account for genuine $2 \to 4$ collinear splittings

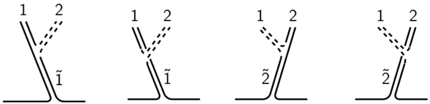
Ferrario Ravasio, Hamilton, AK, Salam, Scyboz, Soyez [2307.11142]

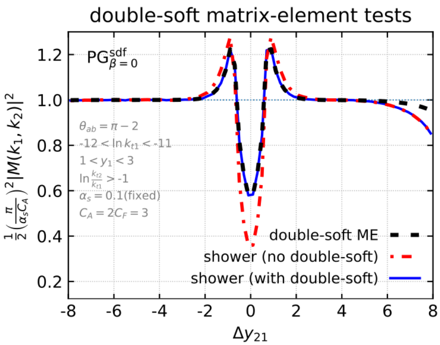
Include double-soft real emissions

- Until recently the inclusion of double-soft emissions in an NLL shower was still an open question
- To get them right we must ensure that any pair of soft emissions with commensurate energy and angles should be produced with the correct ME
- Any additional soft radiation off that pair must also come with the correct ME
- In addition must get the single-soft emission rate right at NLO (CMW-scheme)
- This should achieve NNDL accuracy for multiplicities, i.e. terms $\alpha_s^n L^{2n}$, $\alpha_s^n L^{2n-1}$ and $\alpha_s^n L^{2n-2}$
- and next-to-single-log (NSL) accuracy for non-global logarithms, for instance the energy in a rapidity slice, $\alpha_s^n L^n$ and $\alpha_s^n L^{n-1}$ (albeit only at leading-N_C for now)

Ferrario Ravasio, Hamilton, AK, Salam, Scyboz, Soyez [2307.11142]

The double-soft ME



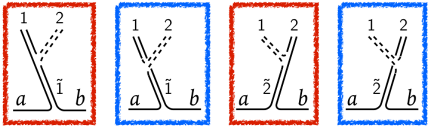


- For now we have focused on PanGlobal
- Any two-emission configuration in a dipole-shower comes with up to four histories (for PanLocal this would in fact be eight)
- We accept any such configuration with the true ME divided by the shower's effective double-soft ME summed over all histories that could have lead to that configuration.

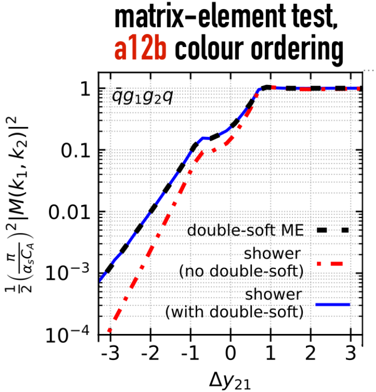
$$P_{\text{accept}} = \frac{|M^2_{\text{DS}}|}{\sum_h |M^2_{\text{shower},h}|}$$

Ferrario Ravasio, Hamilton, AK, Salam, Scyboz, Soyez [2307.11142]

Correcting the colour-ordering



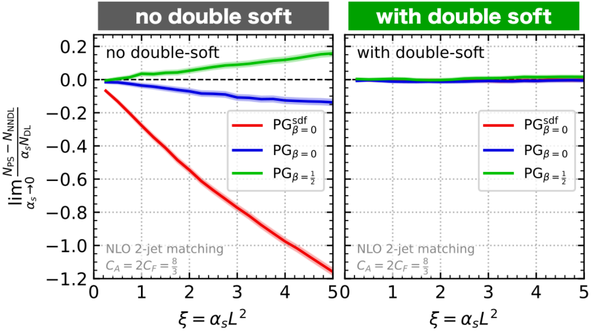
- We have two distinct colour orderings a12b and a21b
- We need to get the relative fractions $F^{(12)}$ and $F^{(21)}$ right in order to ensure that any further emissions are also correct.
- In practice we accept a colour ordering if the shower generates too little of it, and swap them if the shower generates too much (and similarly for $q\bar{q}$ vs gg branchings).



$$P_{\text{swap}} = \frac{F^{(12)}_{\text{shower}} - F^{(12)}_{\text{DS}}}{F^{(12)}_{\text{shower}}}$$

Ferrario Ravasio, Hamilton, AK, Salam, Scyboz, Soyez [2307.11142]

Lund Multiplicities at NNDL ($\alpha_s^n L^{2n-2}$)

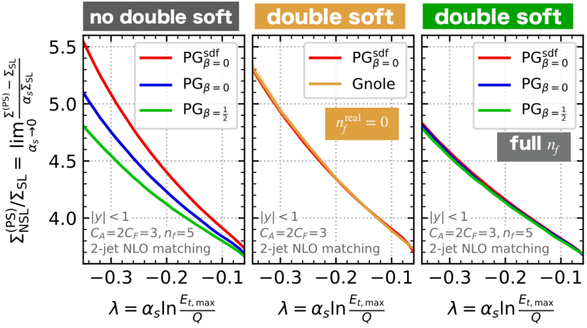


$$\lim_{\alpha_s \to 0} \frac{N_{(PS)} - N_{NNDL}}{\color{red}{\alpha_s} N_{DL}}\bigg|_{\text{fixed } \alpha_s L^2}$$

- Reference NNDL analytic result from Medves, Soto-Ontoso, Soyez [2205.02861]
- We take $\alpha_s \to 0$ limit to isolate NNDL terms. This is significantly more challenging than at NDL due to presence of $1/\alpha_s$ in denominator.
- Showers without double-soft corrections show clear differences from reference (and each other).
- Adding the double-soft corrections brings NNDL agreement.

Ferrario Ravasio, Hamilton, AK, Salam, Scyboz, Soyez [2307.11142]

Energy in a slice at NSL ($\alpha_s^n L^{n-1}$)

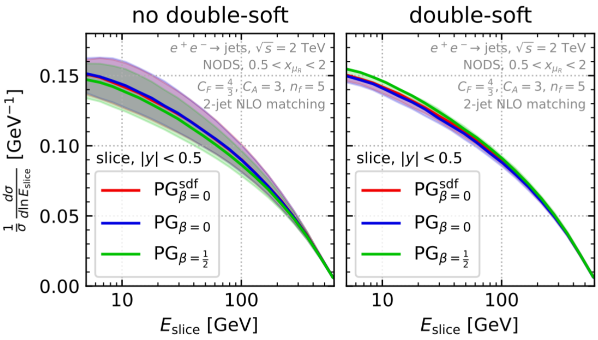


$$\lim_{\alpha_s \to 0} \frac{\Sigma^{(PS)} - \Sigma_{SL}}{\alpha_s}\bigg|_{\text{fixed } \alpha_s L}$$

- Reference NSL from Gnole Banfi, Dreyer, Monni [2111.02413] (see also Becher, Schalch, Xu [2307.02283]).
- We did this test semi-blind: only compared to Gnole after we had agreement between the three PanGlobal variants.
- We have NSL agreement with Gnole (using $n_f^{real} = 0$) and agreement between all showers with full-n_f dependence (first calculation of this kind as a by-product!)

Ferrario Ravasio, Hamilton, AK, Salam, Scyboz, Soyez [2307.11142]

What about pheno?



- We studied energy flow between two hard (1 TeV) jets as a preliminary pheno case
- The three PanGlobal variants are remarkably close without double-soft corrections, but have large uncertainties
- With double-soft corrections we see a small shift in central values but a significant reduction in uncertainties.

Compute triple-collinear ingredients

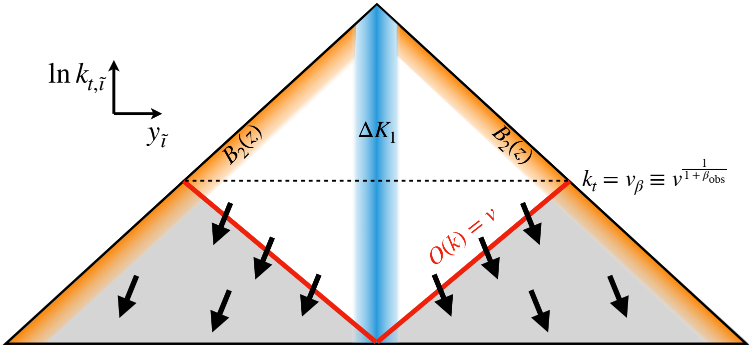
- Double-soft corrections are not by themselves enough to reach NNLL accuracy for event shapes. We also need triple-collinear ingredients (cf. Dasgupta, El-Menoufi [2109.07496], eid. + van Beekveld, Helliwell, Monni, Salam [2307.15734] [2409.08316], eid. + AK [2402.05170] for work in this direction)
- However, it turns out that with the inclusion of real double-soft emissions, only the Sudakov form factor needs to be modified to reach NNLL for event shapes, i.e. we do not need the fullly differential triple-collinear structure
- Taking

$$\alpha_{\text{eff}} = \alpha_s \left[1 + \frac{\alpha_s}{2\pi}\left(K_1 + \Delta K_1(y) + B_2(z)\right) + \frac{\alpha_s^2}{4\pi^2} K_2\right]$$

there are two pieces missing - B_2 which is of triple-collinear origin [2109.07496], [2307.15734] and K_2 (A_3) which is known Banfi, El-Menoufi, Monni [1807.11487], Catani, De Florian, Grazzini [1904.10365]

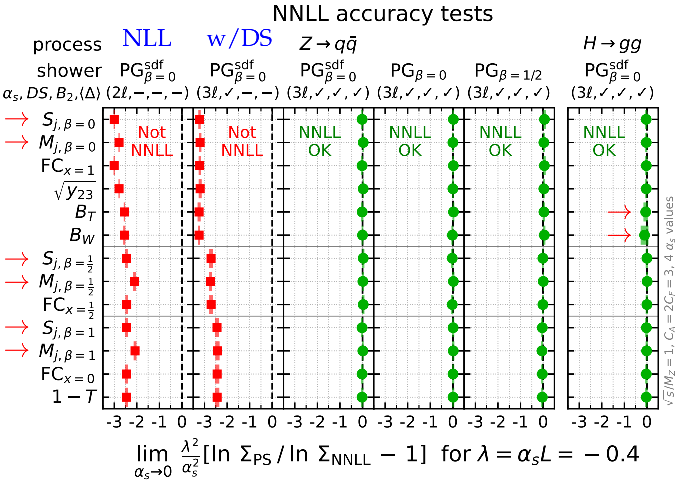
- NB: NLL showers generate spurious $\tilde{B}_2$ and $\tilde{K}_2$ $\rightarrow$ must be compensated

An intuitive picture



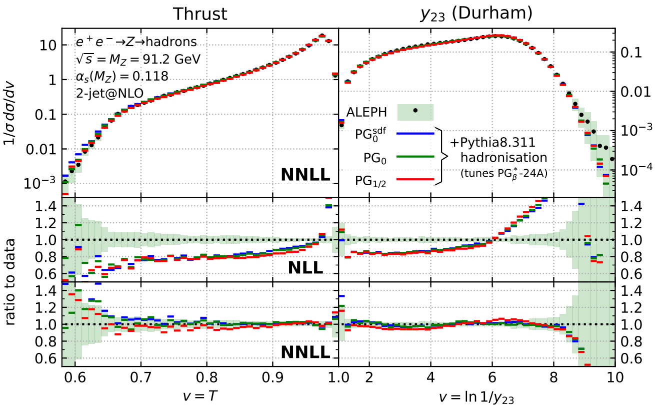
Imagine an emission, $\tilde{\imath}$, sitting anywhere right at the observable boundary (red line). The key observation is that whenever the shower splits $\tilde{\imath} \to 12$, the kinematic variables $(y_{12}, k_{t,12}, z_{12})$ of the resulting pair, do not agree with that of the parent $(y_{\tilde{\imath}}, k_{t,\tilde{\imath}}, z_{\tilde{\imath}})$. Since the Sudakov was computed assuming conserved kinematics of $\tilde{\imath}$, and the observable is computed with the actual kinematics of (12), we have generated a mismatch. We can compute these drifts!

Are we there yet?



- $\rightarrow$: New analytic results, not available in literature van Beekveld, Buonocore, El-Menoufi, Ferrario Ravasio, Monni, Soto-Ontoso, Soyez [in preparation]
- With no NNLL improvements, the coefficient of NNLL difference is significant, $\mathcal{O}(2-3)$, indicating importance of getting NNLL right
- With the inclusion of double-soft, observables with the same β_{obs} align but do still not agree with the analytics
- After inclusion of shifts and B_2 and K_2 we have perfect agreement

Not far now...



Long-standing tension between LEP data and Pythia8 unless using an anomalously large value of $\alpha_s(M_Z) = 0.137$ Skands, Carrazza, Rojo [1404.5630] (also present for PanScales showers)

Inclusion of NNLL brings large corrections with respect to NLL

Agreement with data achieved without anomalously large value of α_s

Beware: no 3j@NLO which is known to be relevant in the hard regions

Residual uncertainties still need to be worked out

Take-away message

Showers with controlled logarithmic accuracy are here

Several groups have reached NLL – PanScales has also reached partial NNLL

NNLL seems important for phenomenology

But so-far only preliminary studies available

Public code available since v0.3 release PanScales [2312.13275]

`https://gitlab.com/panscales/panscales-0.X`

And now for something (completely) different...

The problem of negative weights

1. Negative weights reduce the statistical power of event samples $\rightarrow$ leads to higher computational costs and in extreme cases to systematic errors

Given fraction f of negative-weight events, to reach the same statistical error as for N unit positive-weight events, you need to generate a larger number of events,

$$\frac{N}{(1-2f)^2}.$$

Already at 15% negative weights do we need twice as many events.

CMS [2205.05550]: "The main experimental systematic uncertainties are associated with limited simulation sample sizes, particularly due to large fractions of negatively weighted events in the NLO V+jets samples [...]"

The problem of negative weights

2. They are notoriously difficult to handle in certain ML applications $\rightarrow$ bias results by either throwing away (or take absolute value) or force the use of LO samples

ATLAS [2211.01136]: "To avoid the use of negative weights present in the nominal NLO sample in the training of the multivariate discriminant used to separate SM $t\bar{t}t\bar{t}$ events from background [...], a sample was produced with similar generator settings, but at LO."

CMS [2411.03023]: "However, the binary cross-entropy given by Eq. (2), can become negatively unbounded for negative event weights, making the classification task potentially impossible"

ATLAS [2412.15123]: "Since XGBoost [ML framework] cannot handle negative-weight events, the absolute value of each event weight is used."

The problem of negative weights

3. Although negative weights have to be absent in physical predictions, their presence in intermediate steps points to a profoundly unphysical organisation of the calculation

Are we doing a good enough job if we cannot deliver guaranteed positive predictions?

Origins of negative weights in NLO matching

Two elements need to come out right in NLO matching:

1. The overall normalization must be NLO accurate.
2. The first/hardest emission must be correct at $\mathcal{O}(\alpha_S)$.

In MC@NLO Frixione & Webber [hep-ph/0204244] the second condition is associated with negative weights, whenever the shower overestimates the true real emission matrix element.

In other methods, most notably POWHEG Nason [hep-ph/0409146] but also KrkNLO Jadach, Płaczek, Sapeta, Siódmok, Skrzypek [1503.06849] and MAcNLOPS Nason & Salam [2111.03553], this condition is handled without negative weights.

Aim of ESME (Exponentiated Subtraction for Matching Events): eliminate remaining negative weights associated with 1.

The NLO normalization

For a fixed Born configuration, Φ_B, the NLO normalization is given by

$$\bar{B}(\Phi_B) = B_0(\Phi_B) + \underbrace{V(\Phi_B) + \int R(\Phi_B, \Phi_{rad})\, d\Phi_{rad}}_{\text{relative order } \alpha_s},$$

which is made explicitly finite with a subtraction method

$$\bar{B}(\Phi_B) = B_0(\Phi_B) + \underbrace{V(\Phi_B) + C_{int}(\Phi_B) + \int [R(\Phi) - C(\Phi)]\, d\Phi_{rad}}_{\text{relative order } \alpha_s}.$$

If Φ_B is a perturbative phase space point, then the normalization has to be positive.

The $R - C$ integrand

The main source of negative weights comes from the treatment of

$$\int \underbrace{[R(\Phi) - C(\Phi)]}_{\text{Not pos. definite}} d\Phi_{\text{rad}} .$$

Standard approach to generate a "Born" event

- Choose a Born phase space point Φ_B randomly
- Choose a random real phase space point Φ_{rad} to get a "single-point Monte Carlo" estimate of the integral

$$\bar{B}(\Phi_B) = B_0(\Phi_B) + \underbrace{V(\Phi_B) + C_{\text{int}}(\Phi_B) + \int [R(\Phi) - C(\Phi)] \, d\Phi_{\text{rad}}}_{\text{relative order } \alpha_s} .$$

- Accept with probability $|\bar{B}|/\text{max}$ and assign weight of $\text{sign}(\bar{B})$

Some remedies

There exists an obvious remedy for this problem: *folding* Nason [0709.2085]

Folding

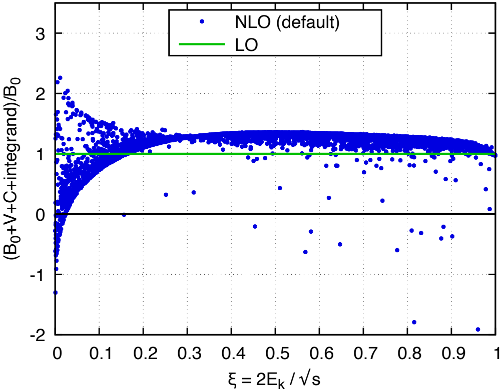
Instead of a single evaluation of the integrand we make n evaluations

But this does not solve the problem of negative weights, it just reduces the fraction of negative weights, at a higher event generation cost.

One alternative is to transform the integrand so that it is less negative – but this is not always easy and still doesn't guarantee a positive definite description. Similar in spirit to "Born spreading" Frederix & Torrielli [2310.04160] and ARCANE Shyamsunda [2502.08052], [2502.08053].

Variable transformation

$$\bar{B}(\Phi_B) = B_0(\Phi_B) + V(\Phi_B) + C_{int}(\Phi_B) + \int [R(\Phi) - C(\Phi)]\, d\Phi_{rad}$$



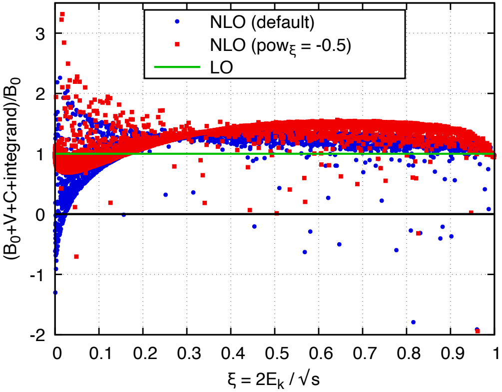
Generate a number of phase space points and plot as a function of one of the radiation variables

Result should be $1 + \mathcal{O}(\alpha_s)$

But coefficient of α_s can be large and negative!

Variable transformation

$$\bar{B}(\Phi_B) = B_0(\Phi_B) + V(\Phi_B) + C_{int}(\Phi_B) + \int [R(\Phi) - C(\Phi)]\, d\Phi_{rad}$$



Transforming the integration variable ξ can help

$$\xi = 1 - z, \quad z \to \sqrt{z}$$

Negative weights remain and not always clear how to perform the transformation (some process dependence)

Toy example for $R - C$

Let us consider $R - C = \alpha_s \left(2 - x^{-2/3}\right)$, such that

$$\bar{B} = 1 + \int_0^1 [R - C]\, dx = 1 - \alpha_s$$

Can we just discard the negative weights?

$$\bar{B}_{>0} = 1 + \int_{R-C>-1}^1 [R - C]\, dx = 1 - \alpha_s + 3\alpha_s^{3/2} + \mathcal{O}(\alpha_s^2)$$

No! That breaks formal NLO accuracy in general.

Key question

Is it possible to evaluate the $R - C$ integral fast & reliably, and be both positive and NLO accurate?

A Sudakov alogorithm

We want to transform the problem, such that we are guaranteed that negative weights are only associated with terms beyond $\mathcal{O}(\alpha_s)$.

Exponentiated subtraction

- Start with normalisation $n_B = 1$ and the max value for k_t (ordering variable)
  Run a loop while $k_t > k_{t,\min}$:
  - Sample $\ln k_t$ from $e^{-M/B_0 \ln 1/k_t}$, where $M = \max(R, C)$,
  - generate random number $0 < r < 1$
  - if $r < \frac{|R-C|}{M}$ then
    $\rightarrow$ if $R > C$: $n_B \rightarrow n_B + 1$
    $\rightarrow$ if $C > R$: $n_B \rightarrow n_B - 1$
- return n_B

$$\langle n_b \rangle = 1 + \int [R(\Phi) - C(\Phi)]/B_0 \, d\Phi_{rad}$$

Discarding negative events

Since each increment or decrement of n_B is associated with a factor α_s, it is clear that to reach $n_B < 0$ one needs at least two powers of α_s.

Keeping the event only if $n_B \geqslant 0$ we guarantee NLO accuracy and positive definitness.

Algorithm can be adapted by multiplying M, R, C by integer p and incrementing n_B by $\pm 1/p$. Gives same $\langle n_B \rangle$ but discarding negative n_B now changes the integral by only α_s^{p+1}.

Many variations possible and in fact we implement something a bit more intricate (but more efficient and gives unweighted events directly)...

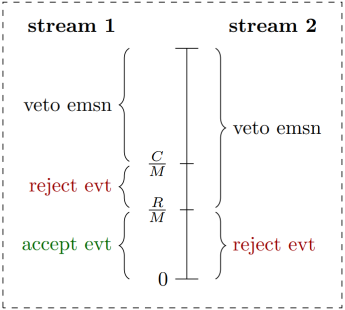
Exponentiated subtraction for Matching Events

Start by generating a Born event according to

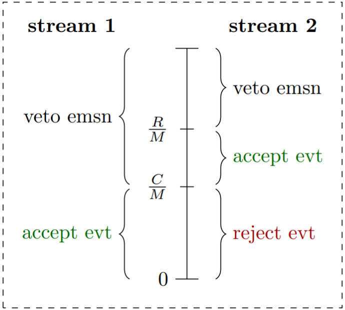
$$\bar{B}_C(\Phi_B) = B_0(\Phi_B) + V(\Phi_B) + C_{\text{int}}(\Phi_B)$$

If this is an overestimate of the true $\bar{B}$ we reject some events, and if it is an underestimate we add extra events. Handled by two separate streams.

ESME, $R < C$



ESME, $R > C$



Wait a minute..

What if $\bar{B}_C(\Phi_B)$ is negative?

Wait a minute..

If $\bar{B}_C(\Phi_B)$ itself is negative, that signals a breakdown of perturbation theory.[2]

In some cases, like Z-production at small p_T, this is a sign of a large logarithm that needs to be resummed.

$$\bar{B} \propto B_0(\Phi_B)(1 - 2\alpha_s C_F/\pi \ln^2 M_Z/p_t)$$

Ideally should be treated through *merging* but we are free to treat this region as we please at $\mathcal{O}(\alpha_s)$. In other cases the physical origin is not as clear, but we still have freedom to deal with it.

[2]We use the NNPDF4.0 MC sets which are positive definite. NNPDF [2406.12961]

Dealing with $\bar{B}_C < 0$

We can write

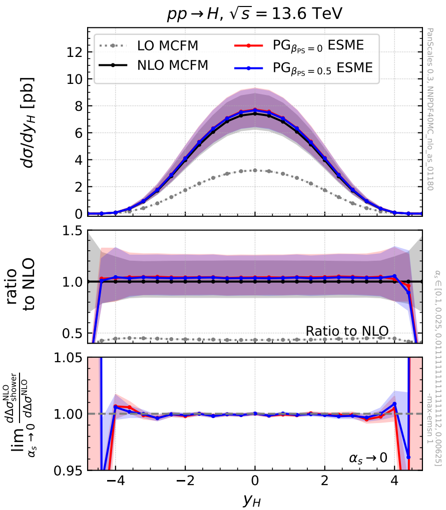
$$\bar{B}_C = B_0[1 - \alpha_s B_{C,1}/B_0] \to B_0[1 - f(\alpha_s B_{C,1}/B_0)]\,,$$

as long as $f(x) = x + \mathcal{O}(x^2)$. If we furthermore pick $f(x) > -1$ we guarantee that $\bar{B}_C$ is positive. In practice we take

$$f(x) = \begin{cases} x & \text{for } x \geqslant 0 \\ \tanh x & \text{for } x < 0\,, \end{cases}$$

This choices ensures that spurious higher-orders are $\mathcal{O}(\alpha_s^3)$ and that large positive K-factors are not modified.

Does ESME work?



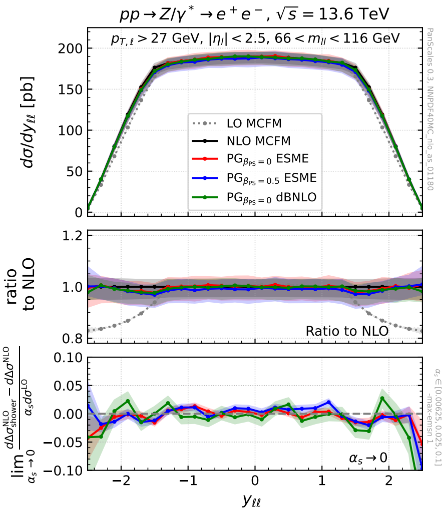
Yes!

$\leftarrow$ Comparison to exact NLO (ggH, NC DY, DIS) [MCFM, disorder]
Campbell & Ellis [hep-ph/9905386]

$\leftarrow$ Ratio to exact NLO (residual α_s^2 contributions visible)

$\leftarrow$ NLO coefficient ($\alpha_s \to 0$)

Does ESME work?



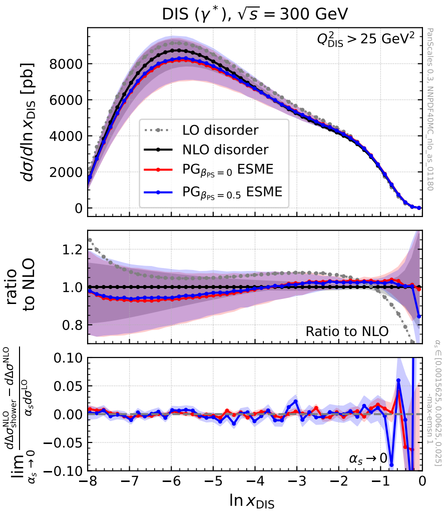
Yes!

← Comparison to exact NLO (ggH, NC DY, DIS) [MCFM, disorder]
Campbell & Ellis [hep-ph/9905386]

← Ratio to exact NLO (residual α_s^2 contributions visible)

← NLO coefficient ($\alpha_s \to 0$)

Does ESME work?



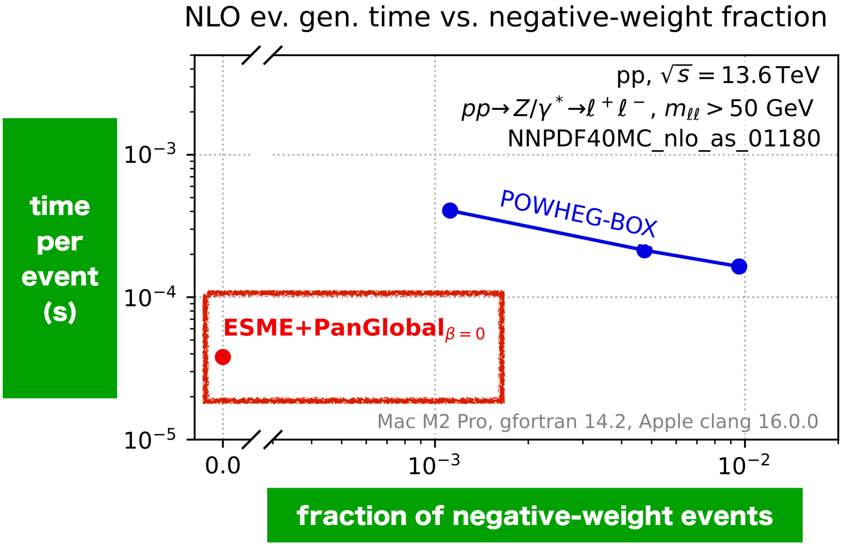
Yes!

← Comparison to exact NLO (ggH, NC DY, DIS) [MCFM, disorder] AK [2401.16964]

← Ratio to exact NLO (residual α_s^2 contributions visible)

← NLO coefficient ($\alpha_s \to 0$)

And it is fast...



Conclusions

Guaranteed positive-definite NLO matching possible

Algorithm simple $\rightarrow$ possible for other groups to try, also for more complex processes

Trade-off is presence of higher order terms

But they are modest and can be controlled (and already present in other methods)

ESME is very efficient

But still need to understand scaling in more complicated processes

Key step to simultaneously accurate and physical pQFT predictions

ESME can be adapted to arbitrary order, e.g. NNLO

BACKUP

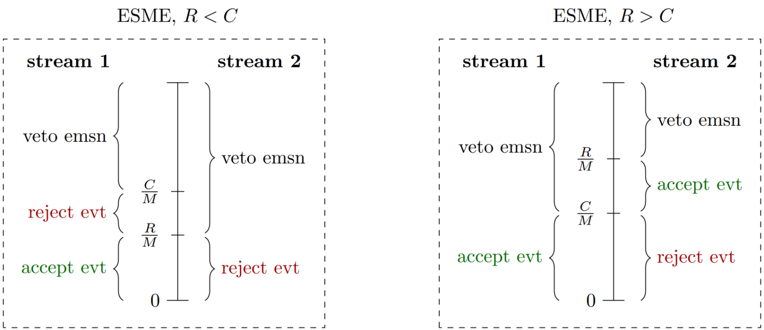


Figure 1: Simple illustration of the different possible actions in the two streams of the ESME algorithm with joint reals and subtractions. The actions are shown separately for the cases $R(\Phi) < C(\Phi)$ (left) and $R(\Phi) > C(\Phi)$ (right). In each case, when summing the two streams, one sees that the "accept evt" action occurs with total weight R/M. One can also verify that the contribution to the total event rate change relative to the $\bar{B}_C$ normalisation is $(R - C)/M$. Recall that the default action in stream 1 (2) is to accept (reject) the event if the shower scale reaches $v_{\min}$ — only when the action is different from the stream's default is the total event rate affected.

Algorithm Stream 1 (ESME) Born + NLO rejection

Generate Born event according to $\bar{B}_C$ distribution and set $v = v_{\max}$
while $v > v_{\min}$ **do**
    generate next v and Φ_2 according to Sudakov with density $\rho(v) d \ln v$, Eq. (3.6)
    generate random number $0 < r < 1$
    if $C(\Phi) > R(\Phi)$ **then**
        if $r > C(\Phi)/M(\Phi)$: veto emission
        else if $r > R(\Phi)/M(\Phi)$: **return** *reject event*
        else: accept emission and **return** *continue shower, accept event*
    else
        if $r > C(\Phi)/M(\Phi)$: veto emission
        else: accept emission and **return** *continue shower, accept event*
return *accept event*

Algorithm Stream 2 (ESME) NLO addition

Generate Born event according to $\bar{B}_C$ (or B_0) distribution and set $v = v_{\max}$
while $v > v_{\min}$ **do**
    generate next v and Φ_2 according to Sudakov with density $\rho(v) d \ln v$, Eq. (3.6)
    generate random number $0 < r < 1$
    if $C(\Phi) > R(\Phi)$ **then**
        if $r > R(\Phi)/M(\Phi)$: veto emission
        else: **return** *reject event*
    else
        if $r > R(\Phi)/M(\Phi)$: veto emission
        else if $r > C(\Phi)/M(\Phi)$: accept emsn, **return** *continue shower, accept event*
        else: **return** *reject event*
return *reject event*

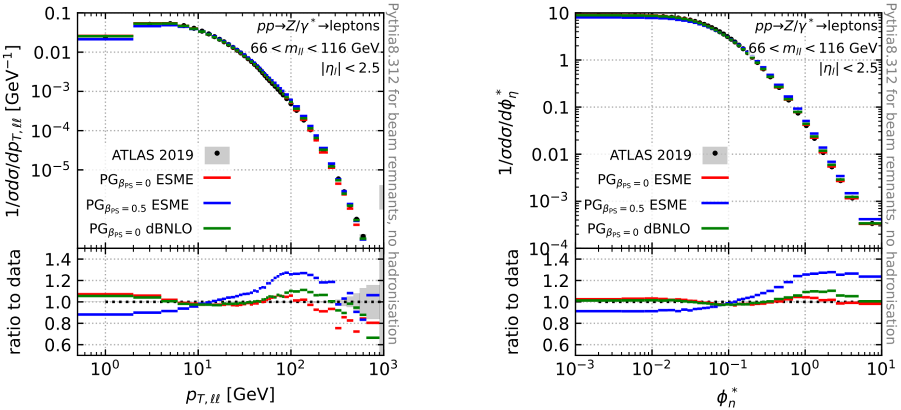


Figure 11: PanScales NLL+NLO matched showers, interfaced with `Pythia` [103], as compared to 13 TeV QED-Born di-lepton data from the ATLAS collaboration [104]. The left-hand plot is for the di-lepton transverse momentum distribution, while the right-hand plot is for the ϕ^*_η variable [105], cf. Eq. (5.1). In the Pythia interface, we include Pythia's primordial transverse momentum but not hadronisation, QED effects or multi-parton interactions.

Slice to subtraction (S2S)

Although we are free to obtain $\bar{B}_C$ however we wish, it is particularly useful if we can represent the countertern in the shower variables $(v, \bar{\eta}, \phi)$.

For $e^+e^- \to q\bar{q}$, and in the limit of small $v < e^{-|L|}$, we have (from slicing)

$$\bar{B}_{PG}(v < e^{-|L|}) = B_0(\Phi_B)\left[1 - \frac{\alpha_s C_F}{2\pi}\left(4L^2 + 6L + \frac{\pi^2}{3} + 2\right)\right],$$

We now construct a counterterm, C, expressed in $\ln v$ and $\bar{\eta}$

$$\frac{C(\Phi)}{B_0(\Phi_B)} d\Phi_{rad} \to \frac{dv}{v} d\bar{\eta} \frac{d\phi}{2\pi} \frac{\alpha_s}{\pi} z P_{gq}(z), \quad \ln z = \bar{\eta} - \bar{\eta}_{max}, \quad 0 < \bar{\eta} < \bar{\eta}_{max} = \ln Q/v,$$

Slice to subtraction (S2S)

$$\bar{B}_{PG}(v < e^{-|L|}) = B_0(\Phi_B)\left[1 - \frac{\alpha_s C_F}{2\pi}\left(4L^2 + 6L + \frac{\pi^2}{3} + 2\right)\right]$$

As in a usual subtraction formalism we now integrate the counterterm above $v > e^{-|L|}$ and obtain

$$\frac{C_{\rm int}(v > Qe^{-|L|})}{B_0(\Phi_B)} = 2\int_{Qe^{-|L|}}^{Q} \frac{dv}{v} \int_0^{\ln Q/v} d\bar{\eta} \int_0^{2\pi} \frac{d\phi}{2\pi} \frac{\alpha_s}{\pi} z P_{gq}(z) = \frac{\alpha_s C_F}{2\pi}\left(4L^2 + 6L + 7\right),$$

which exactly cancels the logarithms in the above.

$$\bar{B}_C = \bar{B}_{PG}(v < Qe^{-|L|}) + C_{\rm int}(v > Qe^{-|L|}) = B_0(\Phi_B)\left[1 + \frac{\alpha_s C_F}{2\pi}\left(5 - \frac{\pi^2}{3}\right)\right].$$

Advantages of S2S

- The counterterm is expressed in the same variables as the shower $\rightarrow$ subtraction formalism directly from the shower
- There is no need to go through the painful exercise of computing the shower in $d = 4 - 2\epsilon$ dimensions
- Can potentially be generalised to higher multiplicity, as long as the slicing computation can be carried out (e.g. N-jetiness, k_t-ness, Lund declustering variables, etc.)
- Obvious path to NNLO

S2S for $pp \to V$

$$\bar{B}_{C}^{\mathrm{PG,DY}} = B_0^{\mathrm{DY}}(\Phi_B)\left[1 + \frac{\alpha_s(\mu_R)}{2\pi}\left(H_{q\bar{q}}^{(1)} + \bar{H}_{q\bar{q}}^{(1)} + \frac{\left((C_{ik}^{(1)} + \bar{C}_{ik}^{(1)}) \otimes f_k\right)(x_i, \mu_F)}{f_i(x_i, \mu_F)} + i \leftrightarrow j\right)\right].$$

$$A_q^{(1)} = 2C_F, \quad B_q^{(1)} = -3C_F, \quad H_{q\bar{q}}^{(1)} = C_F\left(-8 + \frac{7\pi^2}{6}\right), \quad \bar{H}_{q\bar{q}}^{(1)} = C_F\left(1 + 6\ln 2 + \frac{2\pi^2}{3}\right),$$

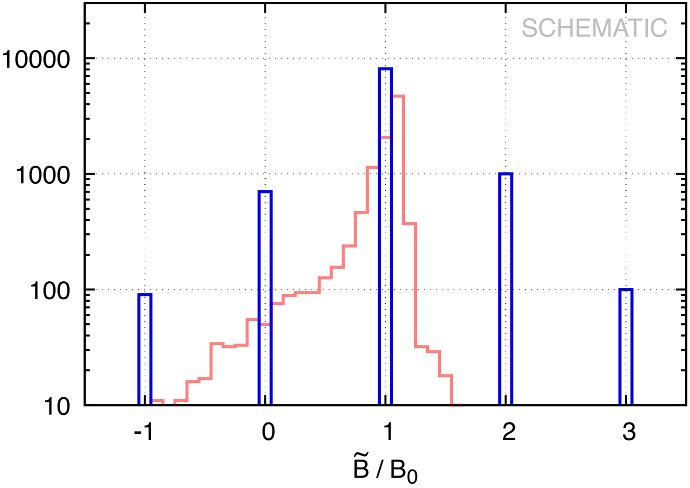
$$C_{ij}^{(1)}(z) = -P_{ij}^{(0),\epsilon}(z) - \delta_{ij}\delta(1-z)C_F\frac{\pi^2}{12} + 2P_{ij}(z)\ln\frac{Q}{\mu_F},$$

$$\bar{C}_{qq}^{(1)}(\bar{z}) = -2\left(p_{qq}(\bar{z})\ln\frac{\bar{z}}{1-\bar{z}}\Theta(\bar{z} > 1/2)\right)_+,$$

$$\bar{C}_{qg}^{(1)}(\bar{z}) = -2p_{qg}(\bar{z})\ln\frac{\bar{z}}{1-\bar{z}}\Theta(\bar{z} > 1/2).$$

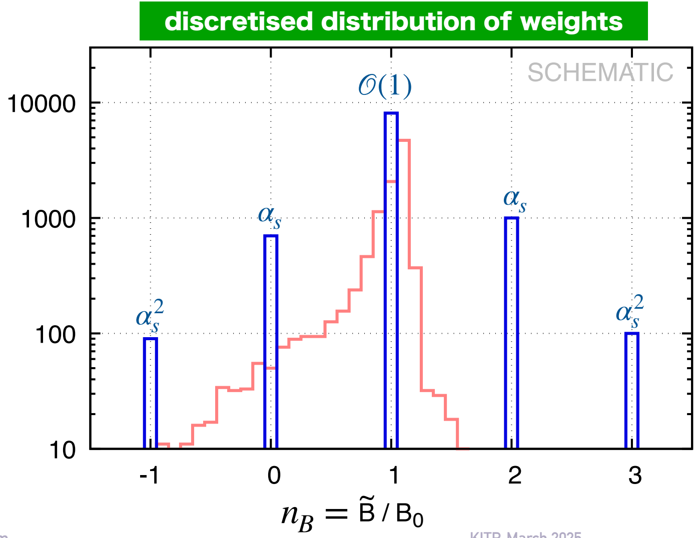
Core idea: map the integral to an event-by event integer

discretised distribution of weights



this can be done in a way that the sum over the distribution gives the exact original answer

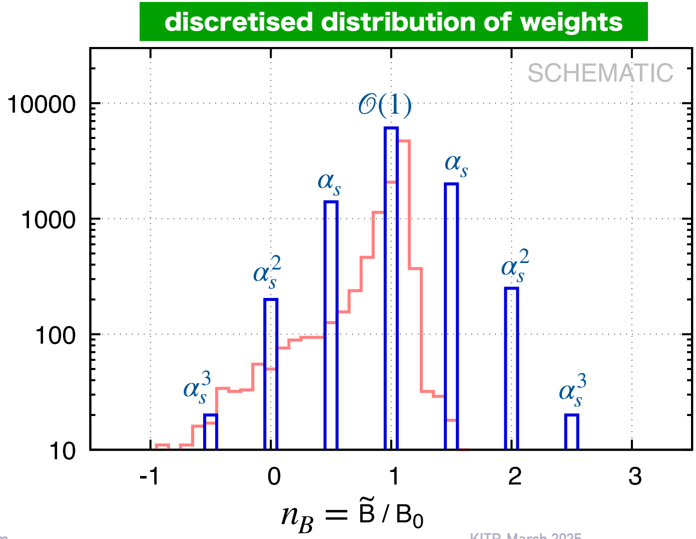
Robust positivity with NLO accuracy (spurious terms from NNLO)



Now if you discard negative-weight events you have a guarantee that you only change the result at NNLO or beyond

Because each decrement of n_B costs a power of α_s

Robust positivity with NLO accuracy (spurious terms from N3LO)



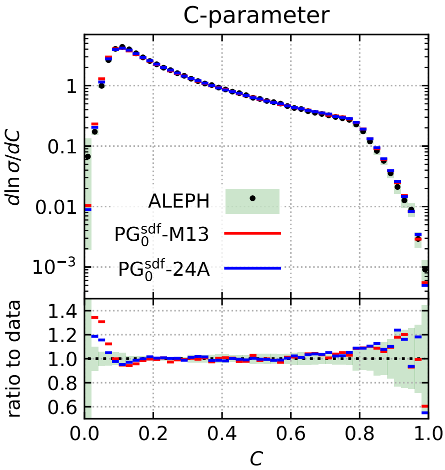
Multiply M, R, C in the algorithm by factor p (here $p = 2$)

Increment n_B by $\pm\frac{1}{p}$

Algorithm gives exactly the same $\langle n_B \rangle$

Keeping only positive-weight events changes integral by just α_s^{p+1}

What about tuning?



Improved agreement with data across a large range of event shapes

Tuning here still rough

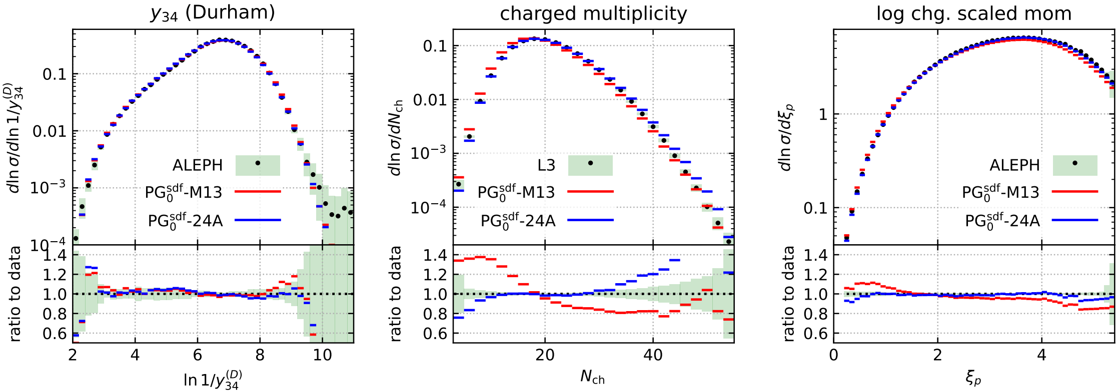
→ We start from the Monash tune (see ref. above) but fix $\alpha_s(M_Z) = 0.118$ (M13)

For our NLL showers this is the tune we use

For the NNLL showers we tune a number of parameters in the string model semi-automatically (24A)

Full tuning exercise still to be done!

What about tuning?

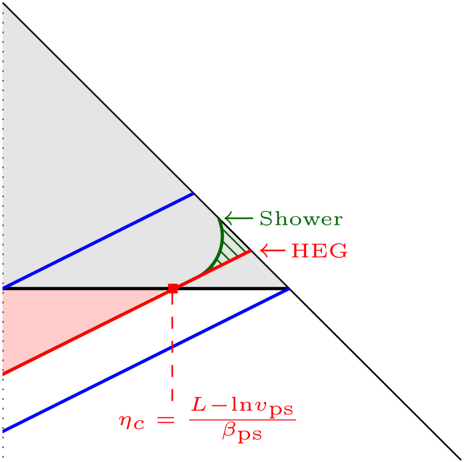


Impact of tune very minor on infrared safe observables, even those that are only NLL accurate

Impact on unsafe observables much larger, bringing good agreement with ALEPH data.

Hamilton, AK, Salam, Scyboz, Verheyen [2301.09645]

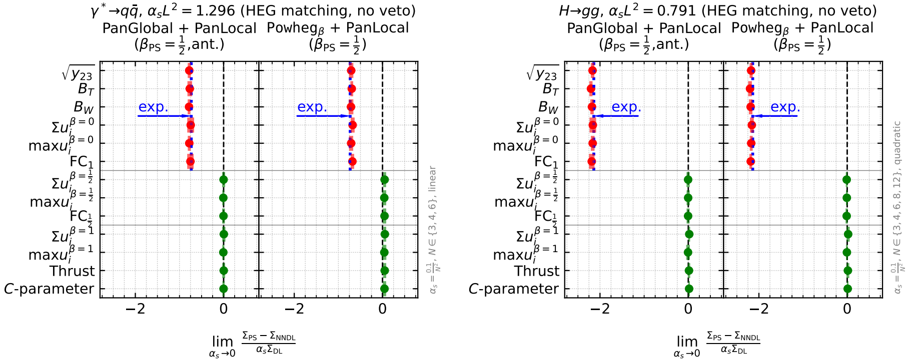
Match without breaking NLL



- We have so far explored the two-body decays $\gamma \to q\,\bar{q}$ and $h \to g\,g$ @ NLO
- For matching schemes that rely on the shower to generate the first emission (such as MC@NLO, KrkNLO, and MAcNLOPS) the matching works more or less out of the box.
- For POWHEG style matchings (including MiNNLO and GENEVA) log accuracy is more subtle to maintain.
- Main concern related to kinematic mismatch between shower and hardest emission generator (in general they are only guaranteed to agree in the soft-collinear region). This issue has been studied in the past Corke, Sjöstrand [1003.2384] but logarithmic understanding is new.

Hamilton, AK, Salam, Scyboz, Verheyen [2301.09645]

HEG without a veto is not NNDL ($\alpha_s^n L^{2n-2}$) accurate

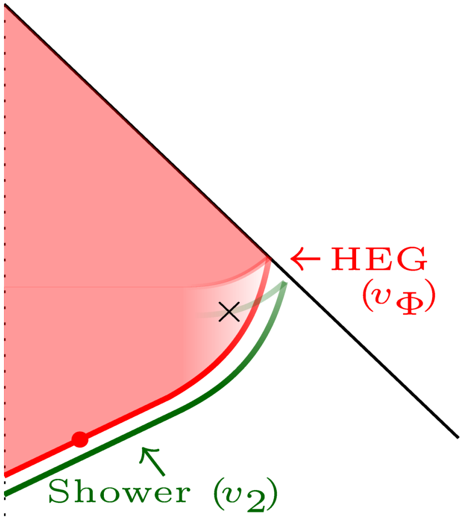


$$\lim_{\alpha_s \to 0} \frac{\Sigma_{\rm PS} - \Sigma_{\rm NNDL}}{\alpha_s \Sigma_{\rm DL}} \Bigg|_{\text{fixed } \alpha_s L^2}$$

Without a veto NLL accurate showers fail our NNDL ($\alpha_s^n L^{2n-2}$) event shape tests. The failure is $\mathcal{O}(1)$, and hence phenomenologically relevant. The dashed blue line indicates the analytically calculated expected value.

Hamilton, AK, Salam, Scyboz, Verheyen [2301.09645]

Further subtleties



- Even when the contours are fully aligned there are issues associated with how dipole showers partition the $g \to gg(q\bar{q})$ splitting function.
- In PanScales we use

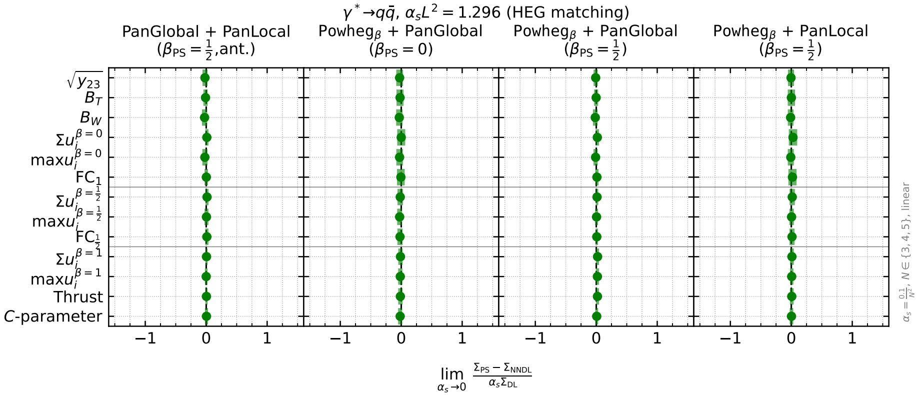
$$\frac{1}{2!}P_{gg}^{\text{asym}}(\zeta) = C_A\left[\frac{1+\zeta^3}{1-\zeta} + (2\zeta-1)w_{gg}\right],$$

such that $P_{gg}^{\text{asym}}(\zeta) + P_{gg}^{\text{asym}}(1-\zeta) = 2P_{gg}(\zeta)$

- This partitioning takes place to isolate the two soft divergences in the splitting function ($\zeta \to 0$ and $\zeta \to 1$), but there is some freedom in how one handles the non-singular part.
- The HEG needs to partition in exactly the same way. Not clear how easy this is in general, in particular in the soft-large angle region.

Hamilton, AK, Salam, Scyboz, Verheyen [2301.09645]

Proper HEG achieves NNDL ($\alpha_s^n L^{2n-2}$) accuracy



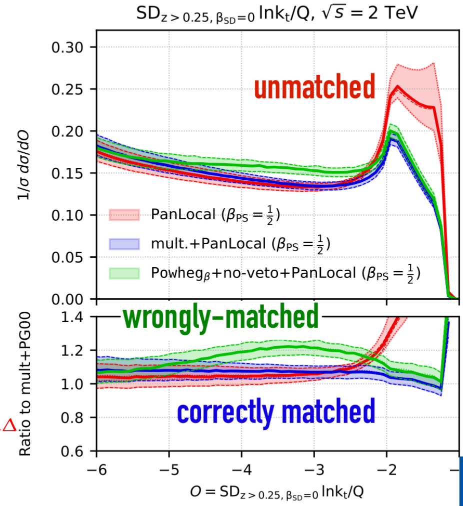
This can be achieved through a standard kinematic veto, as long as shower partioning matches the exact matrix element. A veto however complicates the inclusion of double-soft emissions, since it effectively alters the second emission, complicating the path to further logarithmic enhancement.

Hamilton, AK, Salam, Scyboz, Verheyen [2301.09645]

Phenomenological impact

- Contour mismatch by area $\alpha\Delta$ leads to breaking of NLL and exponentiation
- Correct matching on the other hand augments the shower from NLL to NLL+NNDL for event shapes.
- Impact of NLL breaking terms vary - for SoftDrop they have a big impact due to the single-logarithmic nature of the observable. In particular the breaking manifests as terms with super-leading logs

$$\partial_L \Sigma_{SD}(L) = \bar{\alpha} c\, e^{\bar{\alpha} c L - \bar{\alpha}\Delta} - 2\bar{\alpha} L e^{-\bar{\alpha} L^2} (1 - e^{-\bar{\alpha}\Delta}$$



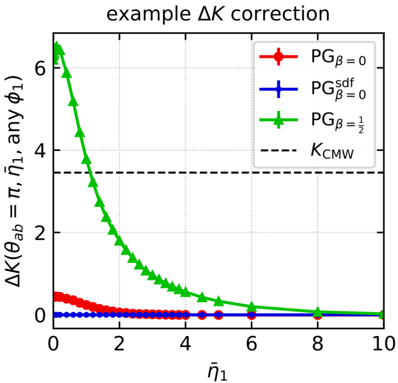
Ferrario Ravasio, Hamilton, AK, Salam, Scyboz, Soyez [2307.11142]

...and associated virtuals!

- The PanScales showers have correct soft emission intensity at NLO in the soft-collinear (sc) region due to the use of the CMW-coupling

$$\alpha_s \to \alpha_s + \alpha_s^2 K_1/2\pi$$

- This in general is not enough the get to soft wide-angle region right and we need to add a ΔK_1 which depends on the rapidity of the single soft emission
- This is related to the fact, that the shower organises its phase space in such a way, that the rapidity of soft pair, y_{12}, does not coincide with the parent rapidity, $y_{\tilde{1}}$.



$$\Delta K_1 = \int d\Phi^{(PS)}_{12/\tilde{1}} |M^{(PS)}_{12/\tilde{1}}|^2 - \int d\Phi^{(PS)}_{12/\tilde{1}_{sc}} |M^{(PS)}_{12/\tilde{1}_{sc}}|^2.$$

Relation between shower and resummation ingredients

It is fairly straightforward to see that at NNLL we only depend on ΔK_1 and B_2 through their respective integrals

$$\Delta K_1^{\text{int}} \equiv \int_{-\infty}^{\infty} dy\, \Delta K_1(y)\,,\; B_2^{\text{int}} \equiv \int_0^1 dz \frac{P_{gq}(z)}{2C_F} B_2(z).$$

These (and K_2) can be related to the drifts in y ($\langle \Delta_y \rangle$), $\ln z$ ($\langle \Delta_{\ln z} \rangle$), and $\ln k_t$ ($\langle \Delta_{\ln k_t} \rangle$) and analytical resummation through

$$\Delta K_1^{\text{int,PS}} = 2\langle \Delta_y \rangle, \quad B_2^{\text{int,PS}} = B_2^{\text{int,NLO}} - \langle \Delta_{\ln z} \rangle, \quad K_2^{\text{PS}} = K_2^{\text{resum}} - 4\beta_0 \langle \Delta_{\ln k_t} \rangle.$$

Using these relations and taking $B_2^{\text{int,NLO}}$ from [2109.07496], [2307.15734] and K_2^{resum} from [1807.11487] one can prove that our showers are NNLL accurate for event-shape observables.