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QCD and advanced Monte Carlo tools

CERN-FNAL HCP summer school – Lecture 4

CERN, 11/6/2011

Summary of lecture 3

- The perturbative part of Event Generators (parton shower) is based on the factorization properties of matrix elements
- Parton showers compute the dominant collinear and soft effects to all orders, effectively resumming them
- Parton showers are inherently collinear — large-p_T emissions are either absent, or wrong
- Rates are computed at the LO
- No reliable estimate of perturbative uncertainties

How can we improve on this?

The current frontier(s)

Go beyond LO (K factors and large-p_T tails)

Done

Go beyond LL

Being done?

How to go beyond LO?

The key issue is to go beyond the collinear approximation

$\Longrightarrow$ use exact matrix elements of order higher than leading

Which ones?

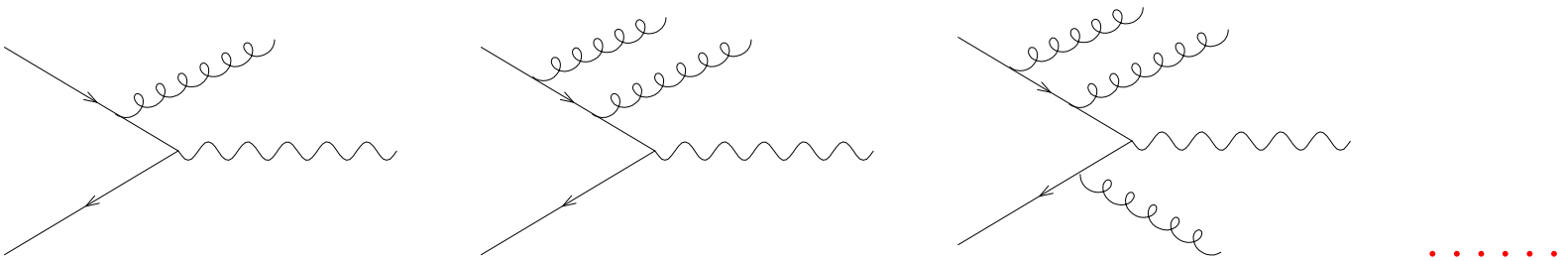
There are two possible choices, that lead to two vastly different strategies:

- Matrix Element Corrections $\longrightarrow$ tree level
- NLOwPS $\longrightarrow$ tree level and loop

I start with MEC

Matrix Element Corrections

Compute (exactly) as many as possible real emission diagrams before starting the shower. Example: W production



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Problems

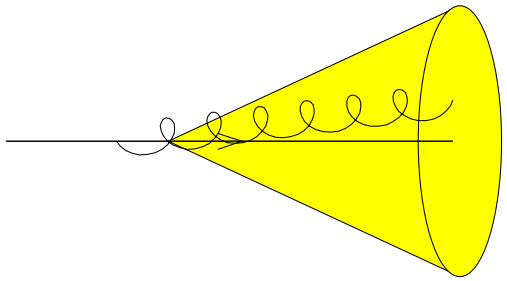
- Double counting (the shower can generate the same diagrams)
- The diagrams are divergent

Solutions

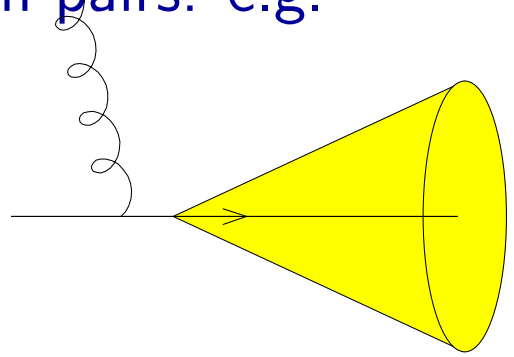
$\longrightarrow$ Catani, Krauss, Kuhn, Webber (2001), Lönnblad (2002), Mangano (2005)
(CKKW, SMPR, CKKW-L, MLM)

What all solutions have in common

- Separate PS- from ME-dominated kinematics regions. This is done by "measuring" the hardness of each parton pairs: e.g.



Soft $\Longrightarrow$ use PS



Hard $\Longrightarrow$ use ME's

- This removes double counting (and divergencies in ME's), but it introduces an unphysical bias, upon which physical predictions depend
- The bias is removed by *at least one* of the following operations

  Modify ME's (through reweighting)

  Choose suitable PS initial conditions (depend on kinematics)

  Forbid emissions/Reject events in the shower phase

CKKW

- Separation criterion: jet k_T clustering algorithm (merge if $d_{ij} < Q^2_{sep}$)
- Reweight ME's with Sudakovs, i.e. the probability that shower could not have generated softer branchings. Sudakovs are LL ones, e.g.

$$\Delta_q(Q_1, Q_2) = \exp\left[-\frac{2C_F}{\pi}\int_{Q_1}^{Q_2} dq \frac{\alpha_S(q)}{q}\left(\log\frac{Q_2}{q} - \frac{3}{4}\right)\right],$$

- Correct the (angular-ordered) shower by *vetoeing* certain emissions (those harder than Q^2_{sep} – hardness is measured by k_T here)
- The latter two steps guarantee that Q^2_{sep} dependence is of NLL

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- Evolution (θ) and merging (k_T) variables not the same: tricky initial conditions, and veto must be forced
- Lack some large-angle soft radiation (should have been emitted by internal lines early in the shower) – a subleading effect?

Accuracy in CKKW

A formal statement has been given only for jet observables in e^+e^- collisions, but is believed to be correct also for hadronic observables

- The separation of the ME- and PS-dominated regions introduces a dependence

$$\sigma_n \sim \alpha_S^{n-2} \sum_k a_k \alpha_S^k \log^{2k} \frac{Q_{sep}^2}{s}$$

  in the n-jet cross section

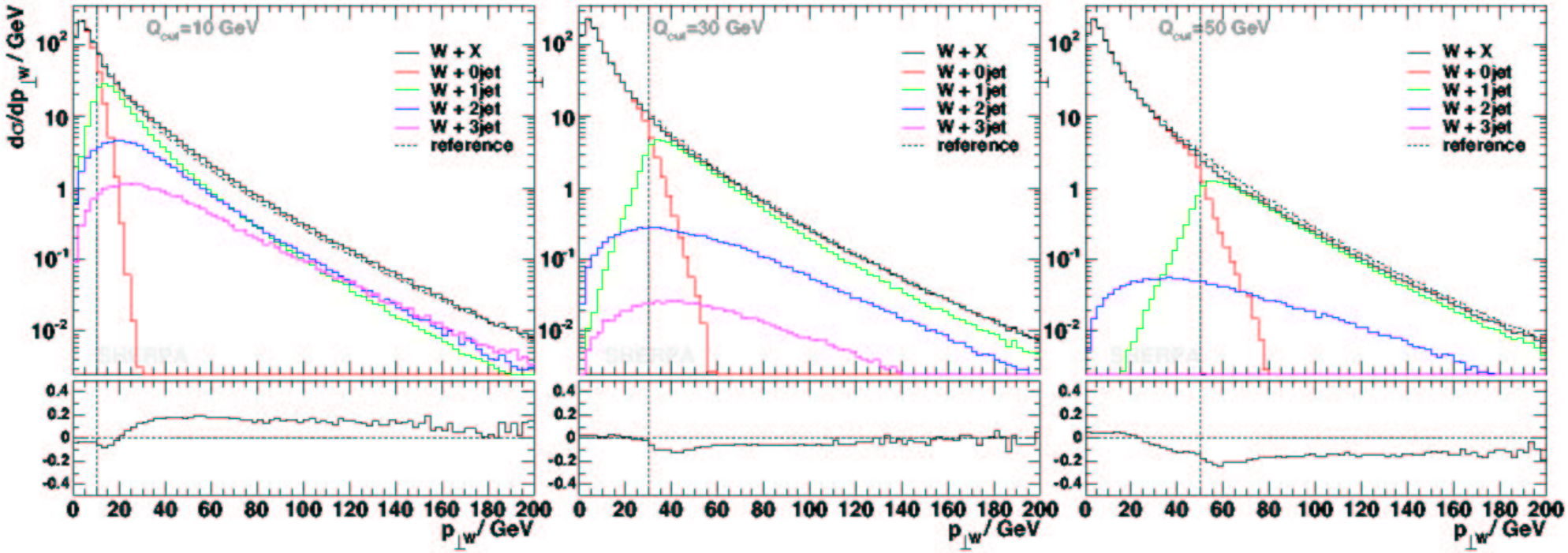
- At the end of the CKKW procedure, this is reduced to

$$\sigma_n \sim \alpha_S^{n-2} \left(\left(\frac{Q_{sep}^2}{s} \right)^a + \sum_k b_k \alpha_S^k \log^{2k-2} \frac{Q_{sep}^2}{s} \right)$$

  ie it is cancelled to NLL accuracy

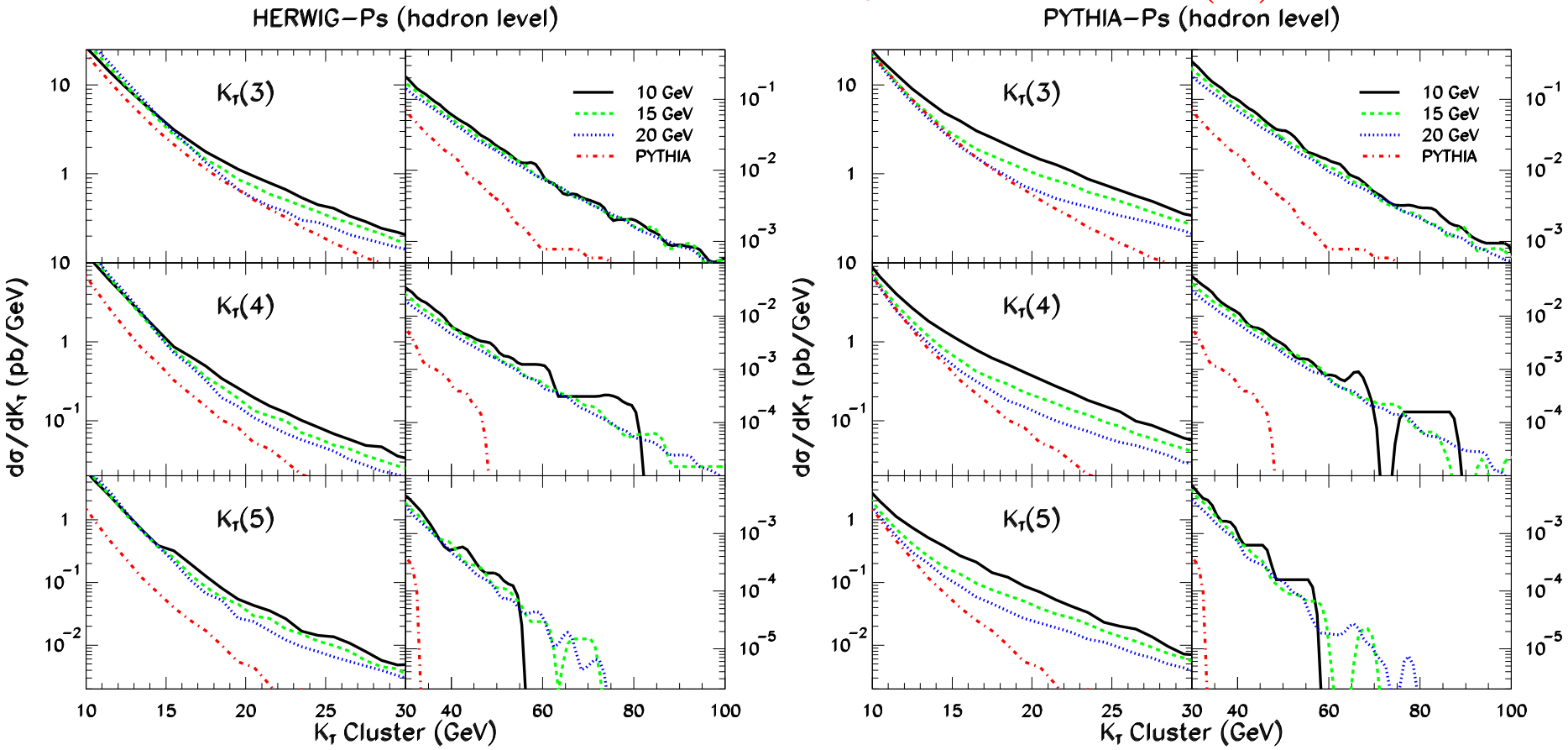
Is this good enough?

Test case: W+jets $\longrightarrow$ $p_T(W)$



- Here $Q_{cut} \equiv Q_{sep}$
- The larger Q^2_{sep}, the smaller the impact of high-multiplicity ME's
- A 20% bias is acceptable, and can be used to tune to the data

Test case: W+jets $\longrightarrow$ $k_T(n)$



- $k_T(n)$ is the value of the resolution scale at which an n-jet configuration becomes an $(n-1)$-jet one
- The dependence on Q^2_{sep} is of the same order as that for $p_T(W)$
- Clear improvements wrt standard parton showers (black vs red lines)

CKKW is an *interpolation* procedure between a PS and the ME's. It defines a fremework, but there is a lot of freedom left, which can be used to reduce unphysical biases on observables

- Clustering algorithm and momentum-recombination scheme
- Sudakov definitions
- Scale choices
- Corrections due to $N < \infty$ (highest-multiplicity ME)

Never forget that the Q^2_{sep} dependence can be reduced but not eliminated. So make sure, before embarking in extensive physics studies, that Q^2_{sep} is properly chosen, and the biases are small

CKKW-like

SMPR (S. Mrenna & P. Richardson)

Apply CKKW to hadronic collisions with Pythia and Herwig

Tests several choices of scales and initial conditions

Use (among others) the same Sudakovs as in the MC

SHERPA (pre-2009)

CKKW except for use of virtuality-order shower

SHERPA (2009)

Use (CS) dipole-type shower, p_T-ordered

Introduce a clustering algorithm that matches shower variables

Use the same Sudakovs as in MC

Add soft radiation where lacking

CKKW-L (Lönnblad)

Implemented in ARIADNE, thus uses dipole shower and p_T ordering

Clustering is done by inverting shower evolution. This implies that intermediate configurations are indistinguishable from shower-generated final states (in CKKW, this is true only up to power-suppressed effects)

Use the same Sudakovs as in the MC

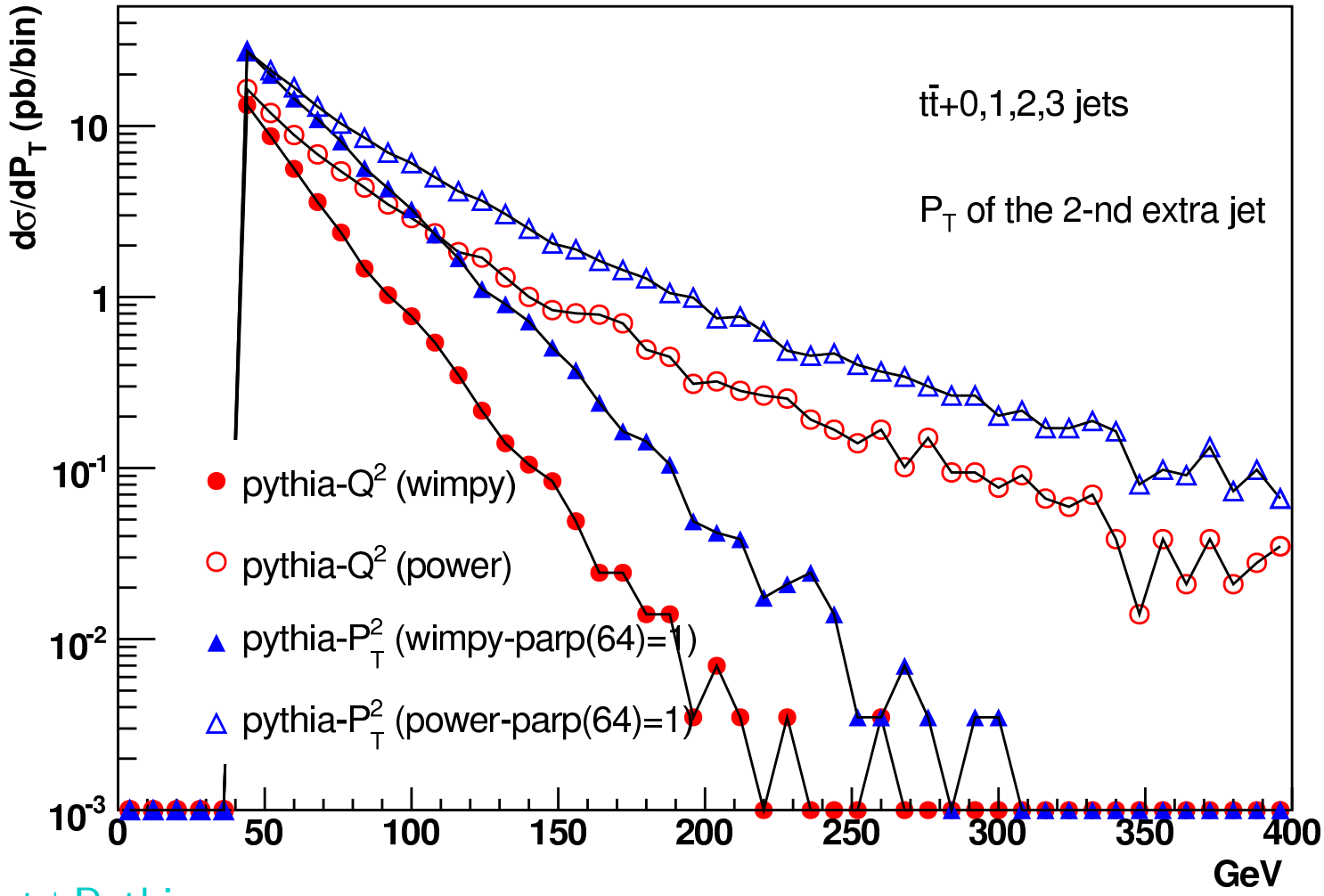
MLM (Mangano)

A cone algorithm is used for clustering

Shower the hard events without vetoeing. Matrix elements are not reweighted

Reconstruct jets after shower. If the number of jet is not equal to the number of original hard partons, throw the event away
(this corresponds to matrix element reweighting and vetoed showers)

Matching at work: before matching

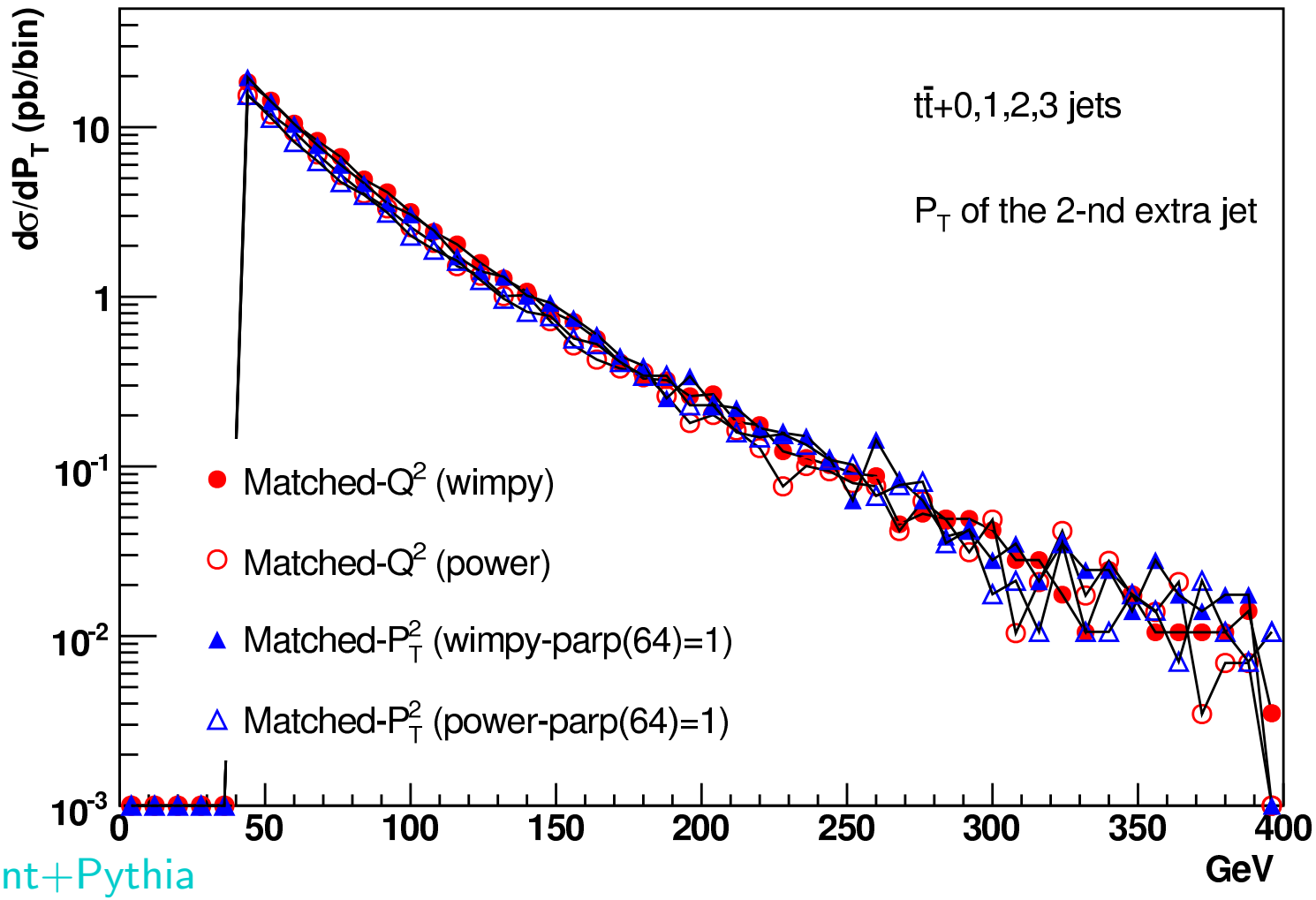


MadEvent+Pythia

OK if you want to fit data, useless to have an idea of how data *will* look like

In other words, good at postdictions, but no predictive power

Matching at work: after matching

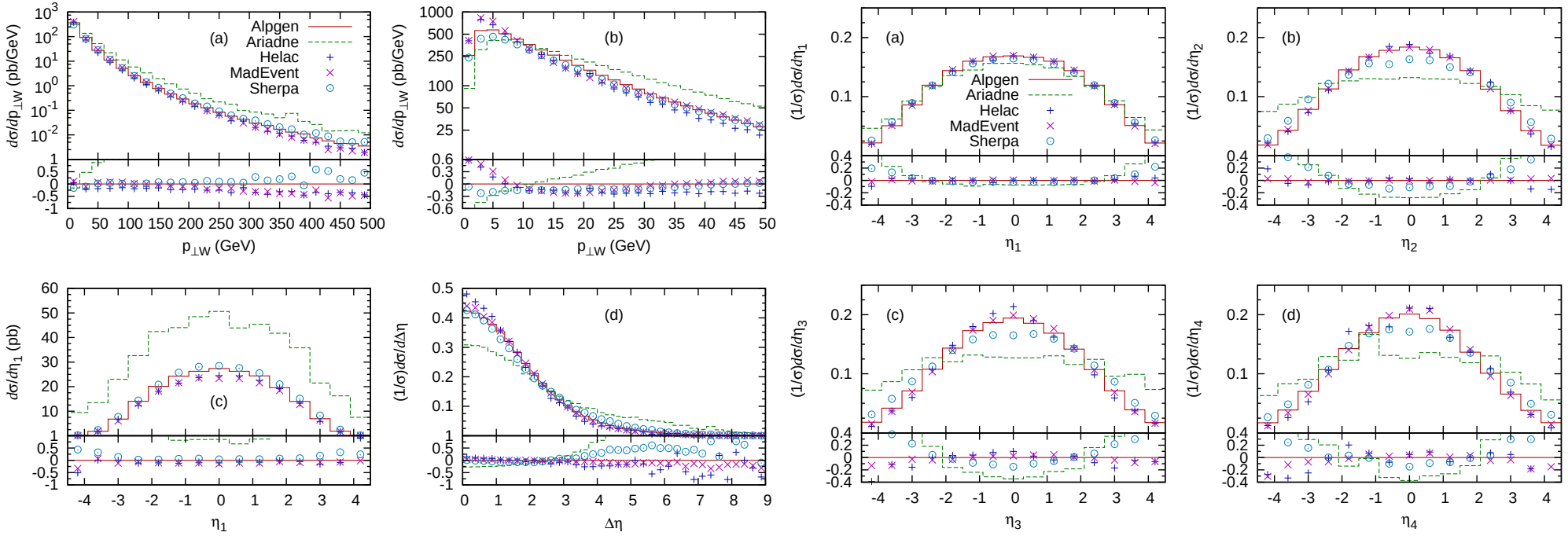


MadEvent+Pythia

A simple reason for this: the physics is right (no collinear approximation used outside the collinear regions)

Is this prediction reliable?

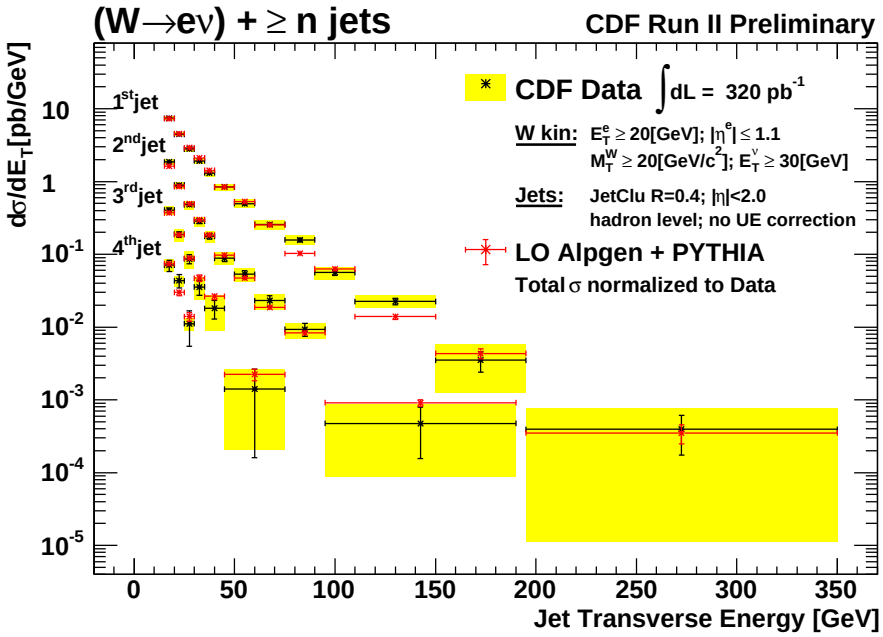
Different matching schemes result in...

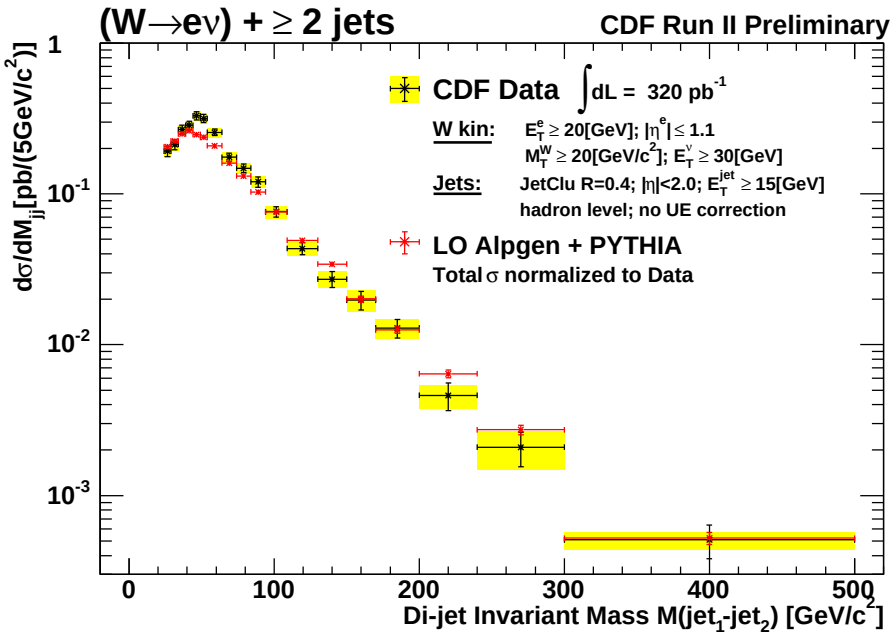


(Alwall *et al.*, 0706.2569)

...reasonably good agreement (10-50%). ARIADNE has the largest differences, but this is more a consequence of lack of proper ISR description than of matching

Comparisons to data





http://www-cdf.fnal.gov/physics/new/qcd/wjets_07/wjets.html

Once the overall normalization is fixed (i.e., one parameter) one obtains a very satisfactory description (which improves that of standard MCs by *orders of magnitude*)

Several other successful comparisons exist (typically, for Z/W+jets) using different codes (SHERPA, MadEvent+MCs,...)

MEC: what to take home

Substantial progress made in the past few years. Main consequence: multi-jet backgrounds not a matter of science fiction any longer

- Never forget to check the merging systematics
- Tuning to data is strongly recommended, and anyhow necessary to figure out the correct normalization: these are LO QCD computation!
- These procedures have been thoroughly tested for W/Z+jets. For other processes, or peculiar observables, systematics can be (much?) larger. Compare predictions from different codes

The use of standalone PYTHIA/HERWIG for multi-jet physics cannot be excused any longer. That's the stone age

Interlude: matrix elements

In order to achieve Matrix Element Corrections, one needs the Matrix Elements...

This is not a problem: a variety of solutions exist, that cover pretty much all needs of (a reasonable...) LHC phenomenology

Matrix element generators for specific processes

Feature a pre-defined list of partonic processes, for which phase-space sampling is optimized

Here's a *non-exahustive* list of codes

- AcerMC
- ALPGEN
- GR@PPA
- VECBOS

There are substantial differences in the number of processes simulated, and in the techniques used to compute the matrix elements!

Phase-space sampling typically optimized process-by-process, to improve unweighting efficiency

Matrix element generators for arbitrary processes

Compute the matrix elements for any process given in input by the user (sort of automated matrix element generator authors...)

- AMEGIC++
- CompHEP
- Grace
- HELAC-PHEGAS
- MadEvent/MadGraph

On average, the largest number of external legs is smaller than that obtained with MEGs for specific processes. Beyond-SM capabilities are constantly being added to these codes

Phase-space sampling (where present) cannot be optimized process-by-process. Adaptive importance sampling techniques are used instead

X-sects (pb)	Number of jets						
$e^-\bar{\nu}_e + n$ QCD jets	0	1	2	3	4	5	6
ALPGEN	3904(6)	1013(2)	364(2)	136(1)	53.6(6)	21.6(2)	8.7(1)
AMEGIC++	3905(4)	1014(3)	370(2)				
CompHEP	3947.4(3)	1022.4(5)	364.4(4)				
GR@PPA	3906.37 (4)	1046.85 (5)					
HELAC/PHEGAS/JetI	3786(81)	1021(8)	361(4)	157(1)	46(1)		
MadEvent	3902(5)	1012(2)	361(1)	135.5(3)	53.6(2)		

X-sects (pb)	Number of jets				
$e^-\bar{\nu}_e + b\bar{b} + n$ QCD jets	0	1	2	3	4
ALPGEN	9.34(4)	9.85(6)	6.82(6)	4.18(7)	2.39(5)
AMEGIC++	9.42(5)	9.92(10)			
CompHEP	9.415(5)	9.91(2)			
HELAC/PHEGAS/JetI	9.88(11)	12.68(9)			
MadEvent	9.32(3)	9.74(1)	6.80(2)		

Good agreement among codes

Capabilities will increase with computer power

How to go beyond LO?

The key issue is to go beyond the collinear approximation

$\Longrightarrow$ use exact matrix elements of order higher than leading

Which ones?

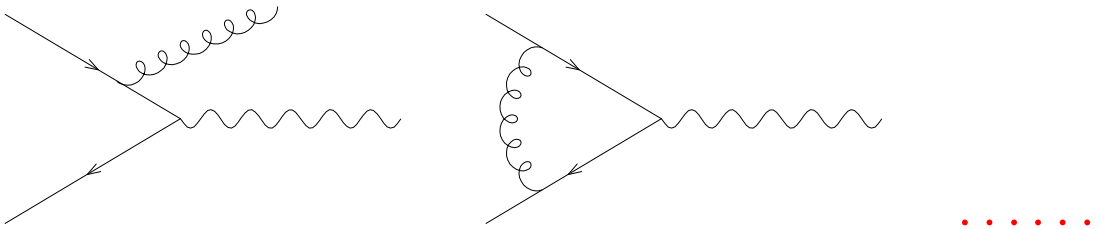
There are two possible choices, that lead to two vastly different strategies:

- Matrix Element Corrections $\longrightarrow$ tree level
- NLOwPS $\longrightarrow$ tree level and loop

I now address the case of NLOwPS

NLOwPS

Compute all the NLO diagrams (and only those) before starting the shower.
Example: W production



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Problems

- Double counting (the shower can generate *some of* the same diagrams)
- The diagrams are divergent

Solution

$\longrightarrow$

Proposals for NLOwPS's

- First working hadronic code (Z): Φ-veto (Dobbs, 2001)
- First correct general solution: MC@NLO (Frixione, Webber, 2002)
- Automated computations of ME's: grcNLO (GRACE group, 2003)
- Absence of negative weights (Nason, 2004; Frixione, Nason, Oleari, 2007) – POWHEG
- Showers with high log accuracy in ϕ_6^3 (Collins, Zu, 2002–2004)
- Within Soft Collinear Effective Theory (Bauer, Schwartz, 2006)
- Showers with quantum interference, colours (Nagy, Soper, 2007–2008)
- Shower and matching with QCD antennae (Giele, Kosower, Skands 2007) – VINCIA
- With analytic showers – GenEvA (Bauer, Tackmann, Thaler, 2008)
- Together with MEC in e^+e^- (Lavesson, Lönnblad, 2008)

Some of these ideas have passed the crucial test of implementation. However, only two codes (MC@NLO and POWHEG) can be used to fully simulate a variety of hadronic processes

NLOwPS vs Matrix Element Corrections

NLOwPS are vastly different from MEC. MEC lack virtual corrections

This forces the use of an unphysical cutoff δ_{sep} in MEC, upon which physical observables depend $\longrightarrow$ matching systematics

NLOwPS are better than MEC since:

+ There is no Q^2_{sep} dependence (i.e., no matching systematics)
+ The computation of total rates is meaningful and reliable

NLOwPS are worse than MEC since:

− The number of hard legs is smaller

- The days of the universal tools are over. Choose the one that best suits your analysis. Typically: small/large number of *extra* legs $\Longrightarrow$ NLOwPS/MEC

Why NLO corrections

- NLOwPS's are the only way in which K-factors can be embedded into MC's (rescaling is WRONG!)

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- Allow a fully-consistent determination of PDF uncertainties (PDF with errors are NLO fits), and of PDFs themselves

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- Realistic hadronization for NLO-accurate predictions
- Allow a fully-consistent determination of PDF uncertainties (PDF with errors are NLO fits), and of PDFs themselves
- Non-trivial dynamics beyond LO ($t - \bar{t}$ asymmetry, FCR vs FEX vs GSP in $b\bar{b}$, $qg \to Wq$, $Wt \leftrightarrow t\bar{t}$ interference, jet algorithms, ...)

MC@NLO

- Compute what the MC does at the first non trivial order, and subtract it from the matrix elements. The resulting short-distance cross sections can be unweighted, and the hard events thus obtained are used as initial conditions for parton showers

- One set of analytical computations per MC (presently, HW and HW++)
- Negative weights
- Strictly identical to MC in soft/collinear regions
- Strictly identical to NLO in hard emission regions;
  all $\mathcal{O}(\alpha_S^{2+b})$ terms not logarithmically enhanced are set equal to zero

NLO and MC computations

- NLO cross section (based on subtraction)

$$\left(\frac{d\sigma}{dO}\right)_{subt} = \int d\phi_{n+1}\Big[\delta(O - O(2 \to n+1))\mathcal{M}^{(r)}(\phi_{n+1}) + \delta(O - O(2 \to n))\Big(\mathcal{M}^{(b+v+rem)}(\phi_n) - \mathcal{M}^{(c.t.)}(\phi_{n+1})\Big)\Big]$$

- MC

$$\mathcal{F} = \mathcal{F}^{(2\to n)}\mathcal{M}^{(b)}(\phi_n)$$

- Matrix elements $\longrightarrow$ normalization, hard kinematic configurations
- δ-functions, $\mathcal{F}^{(2\to n)} \equiv$ showers $\longrightarrow$ kinematic "evolution"

$\Longrightarrow$ How about the replacements

$$\Big(\delta(O-O(2\to n)), \delta(O-O(2\to n+1))\Big) \longrightarrow \Big(\mathcal{F}^{(2\to n)}, \mathcal{F}^{(2\to n+1)}\Big) \; ?$$

Construction of MC@NLO

The naive prescription doesn't work: MC evolution results in spurious NLO terms

$\longrightarrow$ *Eliminate the spurious NLO terms "by hand"*

$$\mathcal{F}_{\text{MC@NLO}} = \mathcal{F}^{(2\to n+1)}\, d\sigma^{(\mathbb{H})}_{\text{MC@NLO}} + \mathcal{F}^{(2\to n)}\, d\sigma^{(\mathbb{S})}_{\text{MC@NLO}}$$

with the two *finite* short-distance cross sections

$$d\sigma^{(\mathbb{H})}_{\text{MC@NLO}} = d\phi_{n+1}\left(\mathcal{M}^{(r)}(\phi_{n+1}) - \mathcal{M}^{(\text{MC})}(\phi_{n+1})\right)$$

$$d\sigma^{(\mathbb{S})}_{\text{MC@NLO}} = \int_{+1} d\phi_{n+1}\left(\mathcal{M}^{(b+v+rem)}(\phi_n) - \mathcal{M}^{(c.t.)}(\phi_{n+1}) + \mathcal{M}^{(\text{MC})}(\phi_{n+1})\right)$$

that feature the *MC subtraction terms*

$$\mathcal{M}^{(\text{MC})} = \mathcal{F}^{(2\to n)}\mathcal{M}^{(b)} + \mathcal{O}(\alpha_S^2\alpha_S^b)$$

POWHEG

- Replace the first MC emission with one generated with a p_T-ordered Sudakov, constructed by exponentiating the *full real matrix element*. Requires a truncated shower to restore the correct pattern of soft emissions for angular-ordered showers

- Short-distance computations independent of MCs
- No negative weights
- Differs from MC in soft/collinear regions if MC is not p_T-ordered. For angular-ordered showers, agreement with MC is restored by truncated showers (up to subleading terms)
- Differs from NLO in hard emission regions by $\mathcal{O}(\alpha_S^{2+b})$ terms; no piece of information on NNLO is used

Construction of POWHEG

Start with an exact phase-space factorization $d\phi_{n+1} = d\phi_n d\phi_r$, and construct

$$\overline{\mathcal{M}}^{(b)}(\phi_n) = \mathcal{M}^{(b+v+rem)}(\phi_n) + \int d\phi_r \left[\mathcal{M}^{(r)}(\phi_{n+1}) - \mathcal{M}^{(c.t.)}(\phi_{n+1})\right]$$

For a *given* p_T, define the *vetoed process-dependent* Sudakov

$$\Delta_R(t_I, t_0; p_T) = \exp\left[-\int_{t_0}^{t_I} d\phi_r' \frac{\mathcal{M}^{(r)}}{\mathcal{M}^{(b)}} \Theta(k_T(\phi_r') - p_T)\right]$$

Obtain hard configurations (to be given to shower as initial conditions) from the short-distance cross section

$$d\sigma_{\rm POWHEG} = d\phi_n \overline{\mathcal{M}}^{(b)}(\phi_n) \left[\Delta_R(t_I, t_0; 0) + \Delta_R(t_I, t_0; k_T(\phi_r)) \frac{\mathcal{M}^{(r)}(\phi_{n+1})}{\mathcal{M}^{(b)}(\phi_n)} d\phi_r\right]$$

which includes Sudakov suppression at $p_T \to 0$

- $k_T(\phi_r)$ will play the role of hardest emission
- The full real matrix element is exponentiated

Attaching (angular-ordered) showers

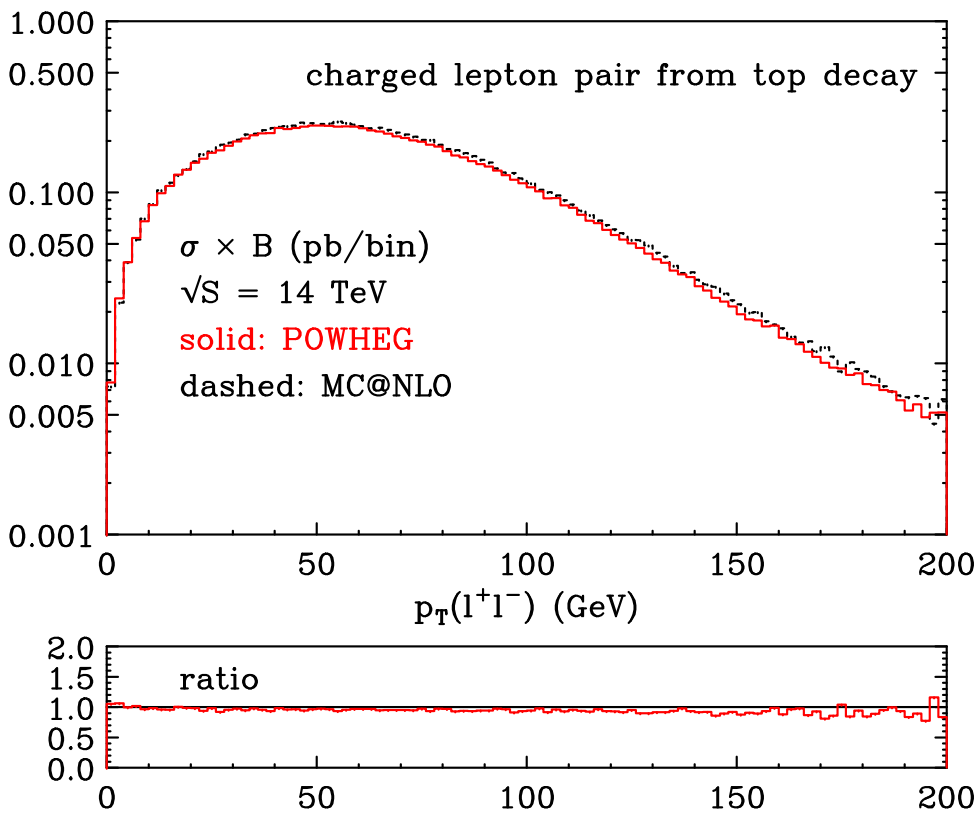
- One wants the matrix-element-generated p_T to be the hardest
  $\Longrightarrow$ veto emissions harder than p_T during shower
- But this screws up colour coherence

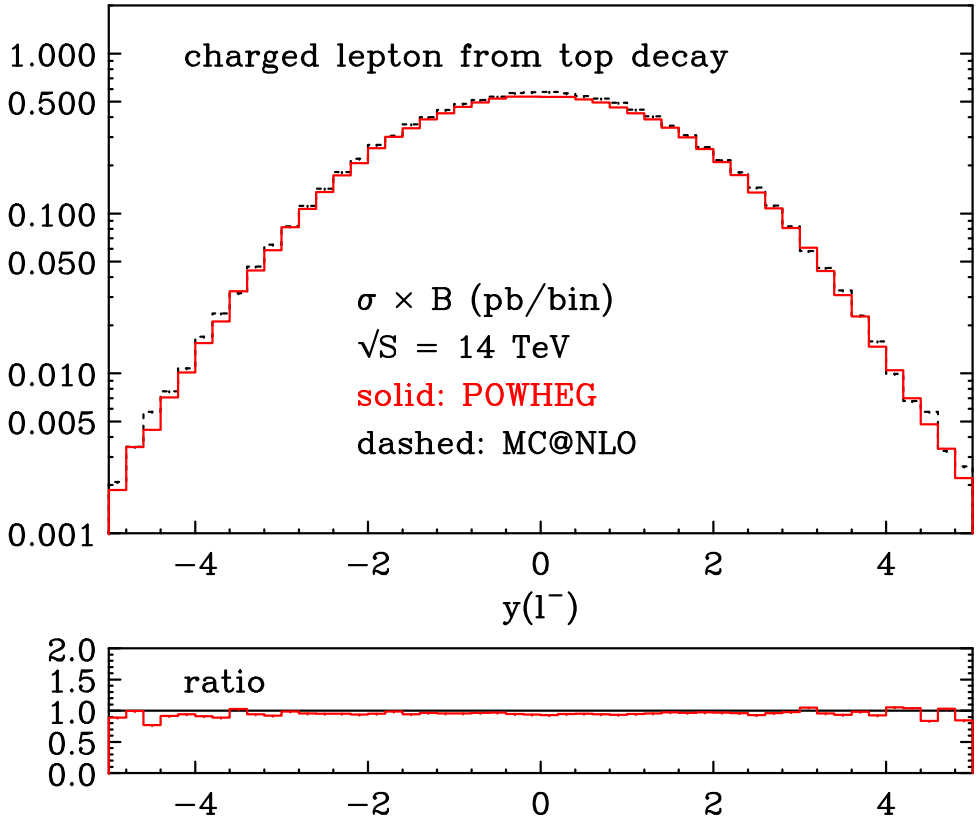
Colour coherence can be restored at the price of a more involved structure

$$\mathcal{F}_{\text{POWHEG}}[t_I; p_T] = \Delta(t_I, t_0) + \int_{t_0}^{t_I} \frac{dt}{t} \int dz \Delta_R(t_I, t; p_T) \frac{\alpha_S}{2\pi} P(z) \times \mathcal{F}_{\text{V}}((1-z)^2 t; p_T)\, \mathcal{F}_{\text{V}}(z^2 t; p_T)\, \mathcal{F}_{\text{VT}}(t_I, t; p_T)$$

- $\mathcal{F}_{\text{V}}(t; p_T)$ are *vetoed* showers. Evolve down to t_0, with all emissions constrained to have a transverse momentum smaller than p_T
- $\mathcal{F}_{\text{VT}}(t_I, t; p_T)$ are *vetoed-truncated* showers. Evolve from t_I down to t (i.e., *not* t_0) along the hardest line. On top of that, they are vetoed

MC@NLO vs POWHEG



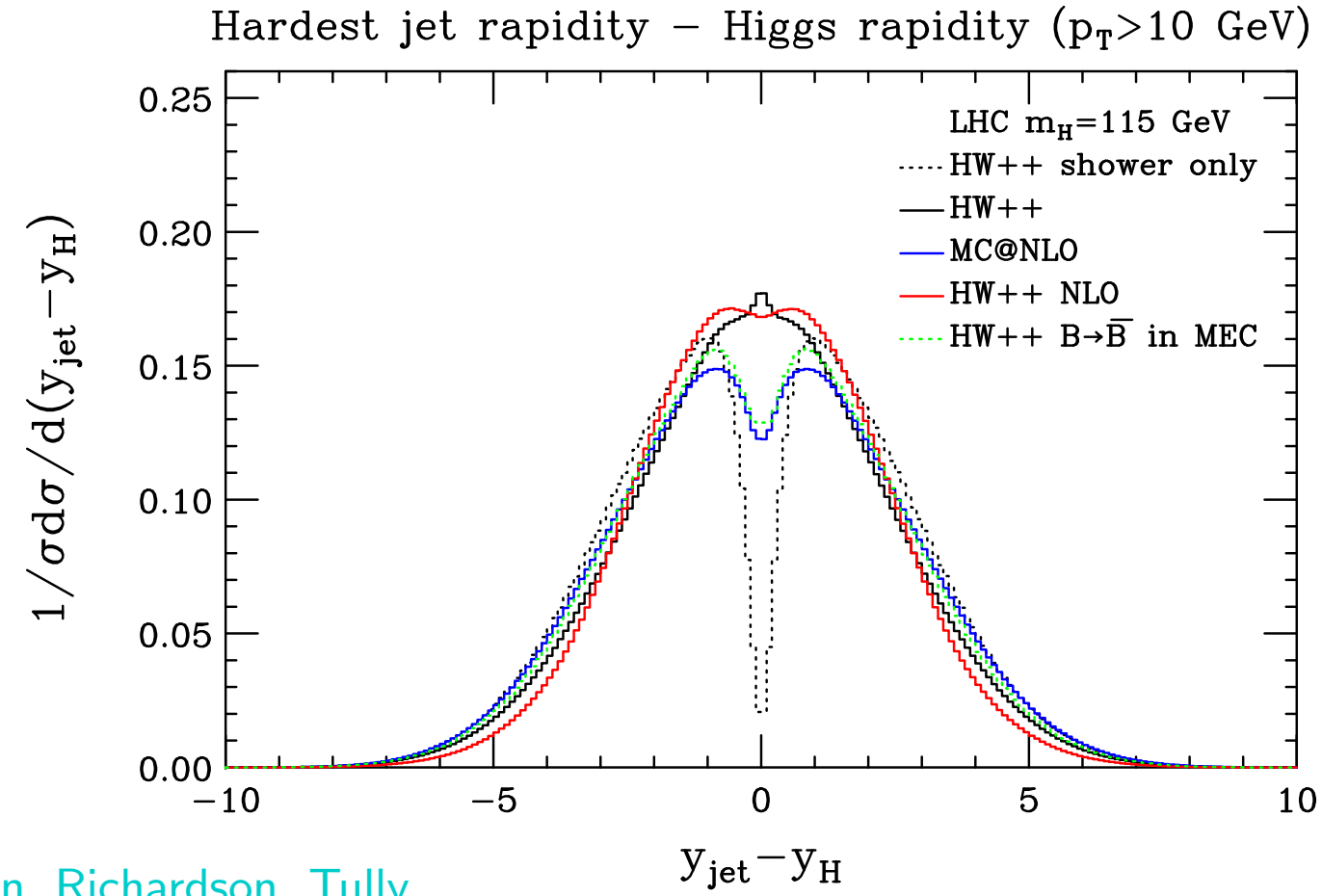


Shown here for lepton observables arising from top decays at the LHC

In the vast majority of cases, extremely good agreement is found

There are a few interesting cases where large differences are found

MC@NLO vs POWHEG: discrepancies



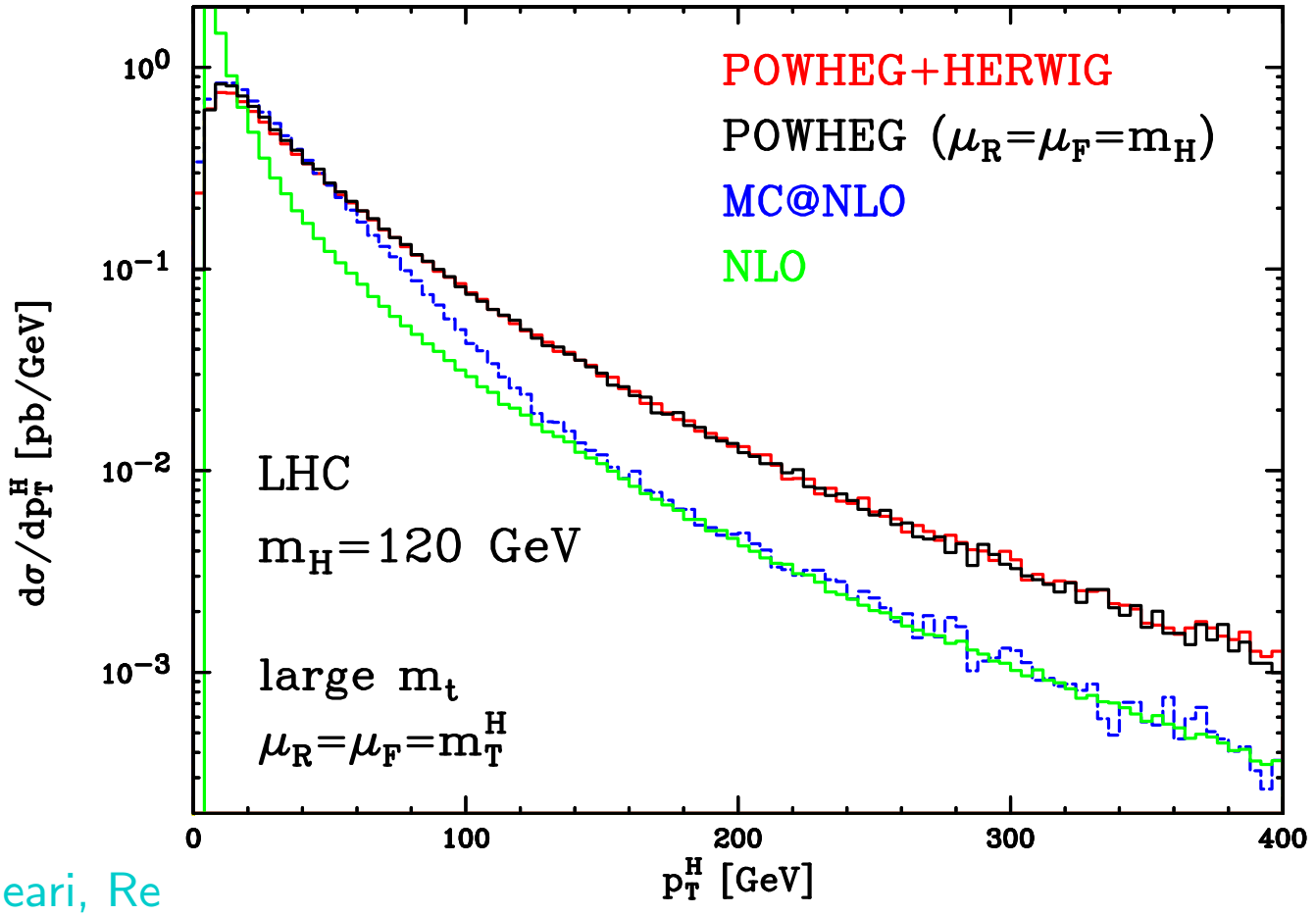
Hamilton, Richardson, Tully

HW/HW++ have dips at $\Delta y = 0$. Likely an artifact of dead zones

MC@NLO fills that dip, via hard radiation

POWHEG fills it much more, owing to extra (spurious) $\mathcal{O}(\alpha_s^4)$ terms

MC@NLO vs POWHEG: discrepancies



Alioli, Nason, Oleari, Re

POWHEG a factor ~ 3 larger than MC@NLO$\equiv$ NLO in the tail

POWHEG result can be decreased by removing part of the real contribution from the exponent $\longrightarrow$

Note: MC@NLO and POWHEG use the *same matrix elements*

$$d\sigma^{(\mathrm{DAMP})}_{\mathrm{POWHEG}} = d\sigma_{\mathrm{POWHEG}} \left(\mathcal{M}^{(r)} \longrightarrow \mathcal{M}^{(r)}_s \right) + \mathcal{M}^{(r)}_f d\phi_n d\phi_r$$

with

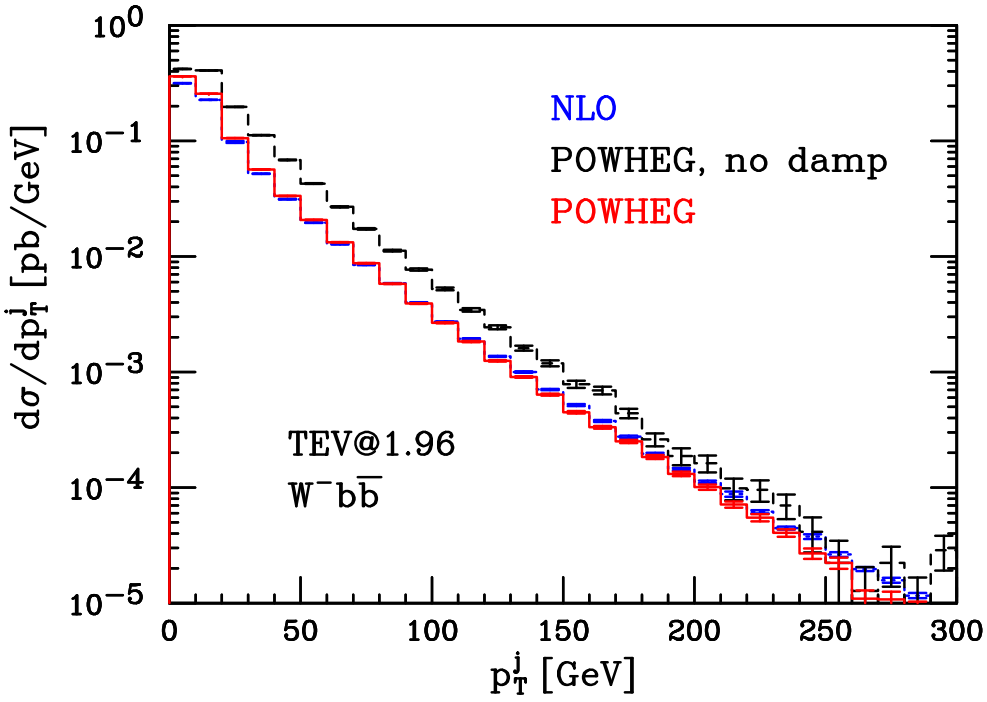
$$\mathcal{M}^{(r)}_s = \mathcal{M}^{(r)} F \,, \qquad \mathcal{M}^{(r)}_f = \mathcal{M}^{(r)} (1 - F)$$

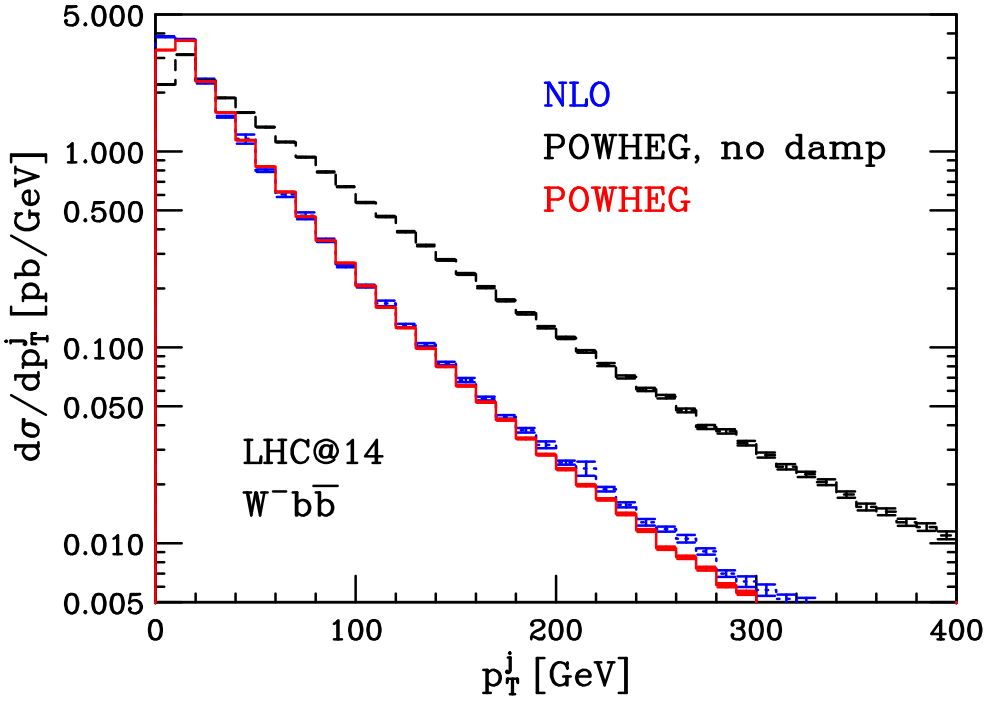
$$0 \leq F = F(\phi_{n+1}) \leq 1$$

$$F \longrightarrow 1 \qquad \text{soft, collinear}$$

The full real matrix element does not exponentiate in QCD. Hence, remove the hardest part of it from the exponent, and bring it downstairs where it belongs. Note that:

$$d\sigma^{(\mathrm{DAMP})}_{\mathrm{POWHEG}} = d\sigma_{\mathrm{POWHEG}} + \mathcal{O}(\alpha_S^{2+b})$$





Oleari, Reina; hardest light jet in $pp \to Wb\bar{b}$

- K factors: 1.9 (Tevatron), 2.74 (LHC)
- The function F is arbitrary. Here, it was specifically chosen to damp hard radiation collinear to the b or $\bar{b}$
- My opinion: F should be considered as theoretical systematics. In cases such as Higgs or $Wb\bar{b}$, it entails a reduced predictive power

MC@NLO vs POWHEG

The two approaches differ by terms of order higher than (N)LL+NLO (ie beyond nominal accuracy). These *may* not be small numerically (although they generally are)

- In MC@NLO, all $\mathcal{O}(\alpha_S^{2+b})$ terms and beyond not logarithmically enhanced (ie, non-MC) are set to zero. In POWHEG, one gets terms of this order, but *not from* an actual NNLO QCD calculation

  Neither code contains any information on non-logarithmic terms of $\mathcal{O}(\alpha_S^{2+b})$ ("NNLO") and beyond

- In MC@NLO the MC generates all non-hard emissions. This is not the case in POWHEG. Technically, this implies an ordering in p_T; thus, double-log accuracy is spoiled if an MC is used that is not ordered in p_T (such as HERWIG). It can be restored by adding a "soft" shower

  Soft showers are only available in HW++, but not in HW6

  Small effects on inclusive variables

Conclusions

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Every theoretical calculation has its limitations.

It is important to understand them, in order to make an educated decision on whether the results can be sensibly used in the context of a given analysis, or need to be improved