Matching & Merging

Rikkert Frederix

Lund University

MCnet School 2021, Beijing, June 28 - July 2, 2021

Contents

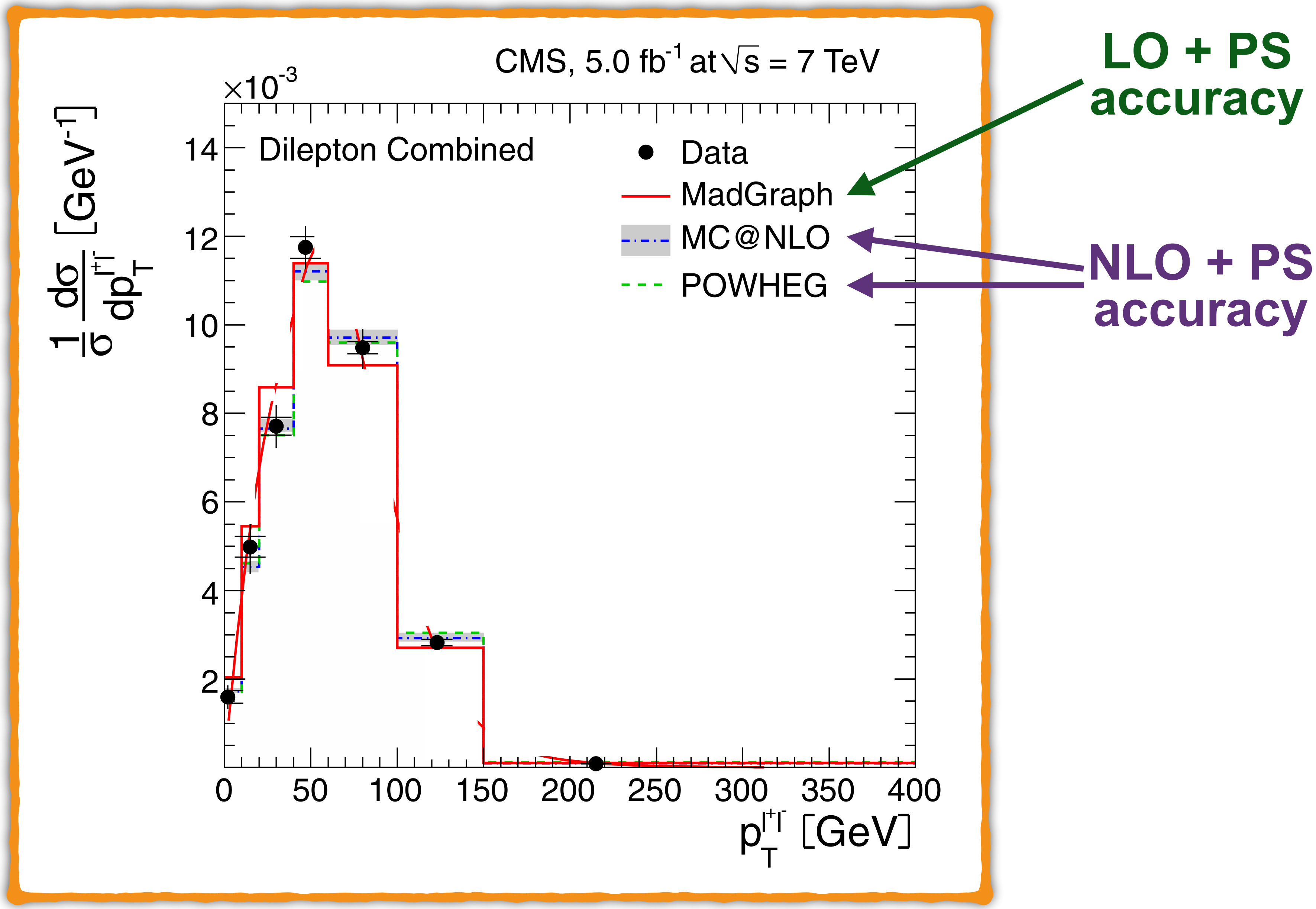
- Quantitative predictions for LHC collisions
  - **Match** NLO matrix elements to Parton Showers
  - **Merge** various multiplicity matrix elements consistently

- Disclaimer: many formulas presented in these lectures are more "schematically correct" than with all details included.

Need for NLO

- Flexible tools available at NLO, the experimental analyses benefit a various ways:
  - NLO predictions predict rates much more precisely
  - Reduced theoretical uncertainties due to meaningful scale dependence
  - Shapes are better described
  - Correct estimates for PDF uncertainties
  - Even data-driven analyses might benefit: smaller uncertainty due to interpolation from control region to signal region
- These accurate theoretical predictions are particularly needed for
  - searches of signal events in large backgrounds samples and
  - precise extraction of parameters (couplings etc.) when new physics signals have been found

Quantitative predictions



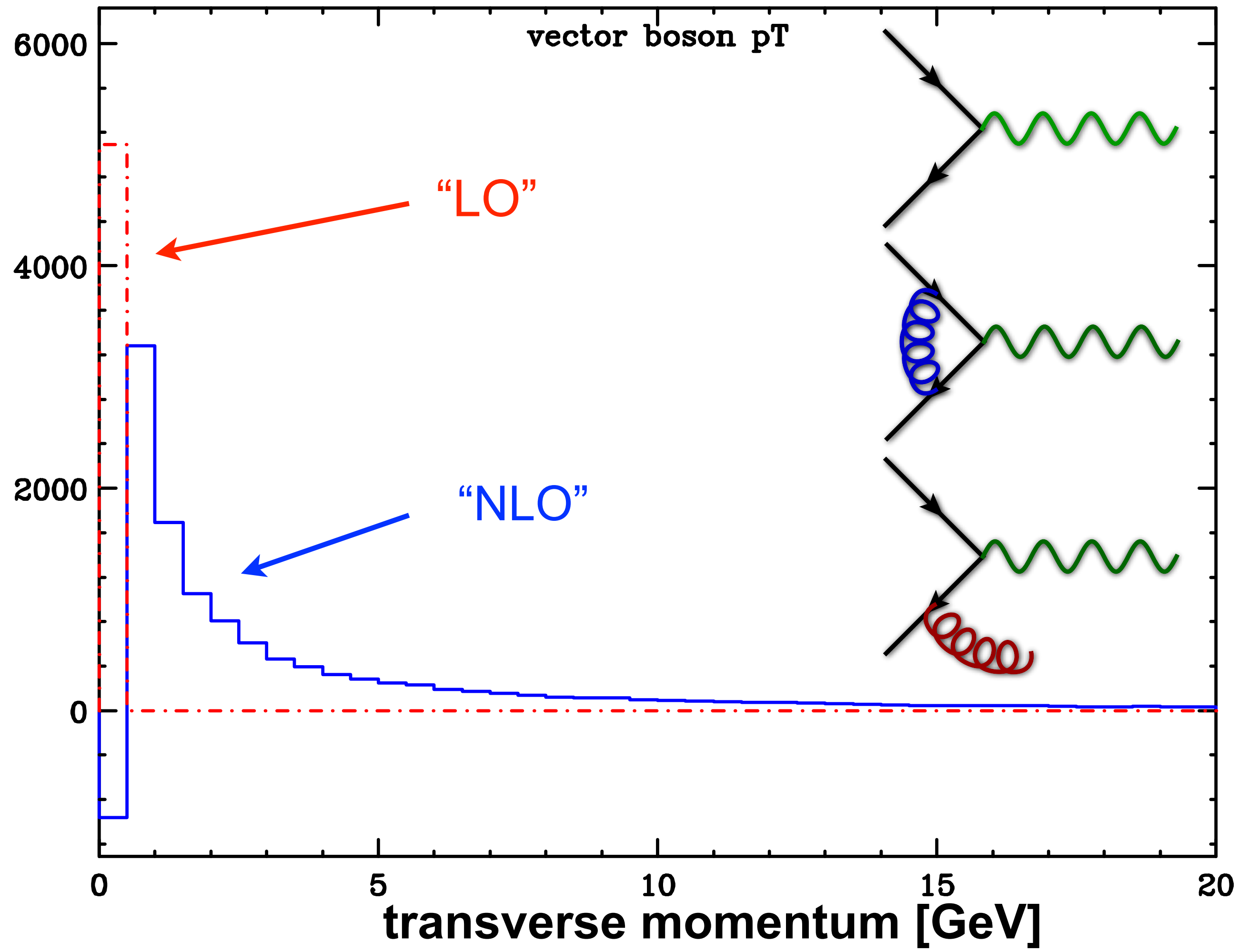
For precise, quantitative comparisons between theory and data, (at least) Next-to-Leading-Order corrections are a must

improving MC’s

- Parton shower MC programs are only correct in the soft-collinear region. Hard radiation cannot be described correctly
- There are two ways to improve a Parton Shower Monte Carlo event generator with matrix elements:
  - NLO+PS matching: Include full NLO corrections to the matrix elements to reduce theoretical uncertainties in the matrix elements. The real-emission matrix elements will describe the hard radiation
  - ME+PS merging: Include matrix elements with more final state partons to describe hard, well-separated radiation better

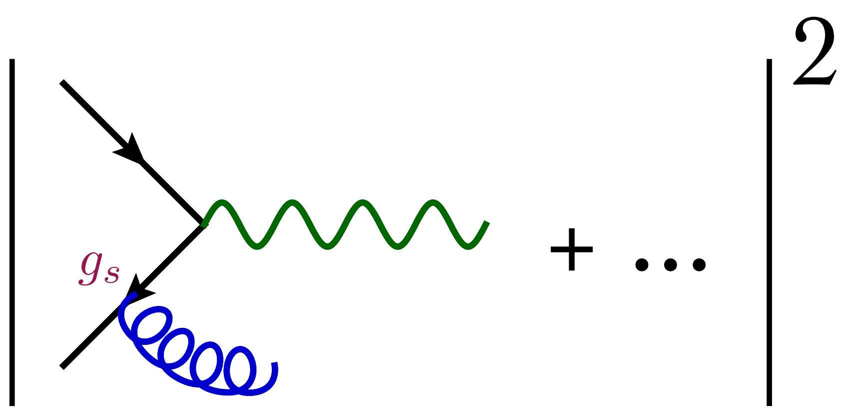
NLO+PS matching

Limitations of Fixed Order calculations



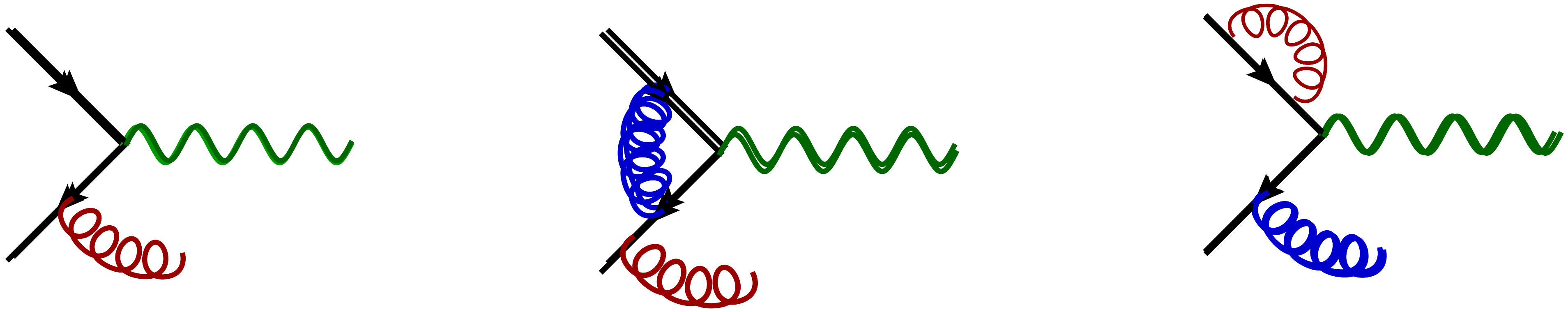
- In the small transverse momentum region, this calculation breaks down (it's even negative in the first bin!), and anywhere else it is purely a LO calculation for V+1j

At NLO



- We have to integrate the real emission over the **complete** phase-space of the one particle that can go soft or collinear to obtain the infra-red poles that will cancel against the virtual corrections
- Hence, we cannot introduce a "cut" that says that:
  - hard radiation needs to be described by the matrix elements
  - and soft radiation by the parton shower
- We have to invent a new procedure to match NLO matrix elements with parton showers

Naive (wrong) approach



- In a fixed order calculation we have contributions with *m* final state particles and with *m*+1 final state particles

$$\sigma^{\rm NLO} \sim \int d^4\Phi_m\, B(\Phi_m) + \int d^4\Phi_m \int_{\rm loop} d^dl\, V(\Phi_m) + \int d^d\Phi_{m+1}\, R(\Phi_{m+1})$$

- We could try to shower them independently
- Let $I^{(k)}_{\rm MC}(O)$ be the parton shower spectrum for an observable O, showering from a k-body initial condition
- We can then try to shower the *m* and *m*+1 final states independently

$$\frac{d\sigma_{\rm NLOwPS}}{dO} = \left[d\Phi_m\left(B + \int_{\rm loop} V\right)\right] I^{(m)}_{\rm MC}(O) + \left[d\Phi_{m+1} R\right] I^{(m+1)}_{\rm MC}(O)$$

Parton shower operator

$$\frac{d\sigma_{\rm NLOwPS}}{dO} = \left[d\Phi_m(B + \int_{\rm loop} V)\right] I_{\rm MC}^{(m)}(O) + \left[d\Phi_{m+1} R\right] I_{\rm MC}^{(m+1)}(O)$$

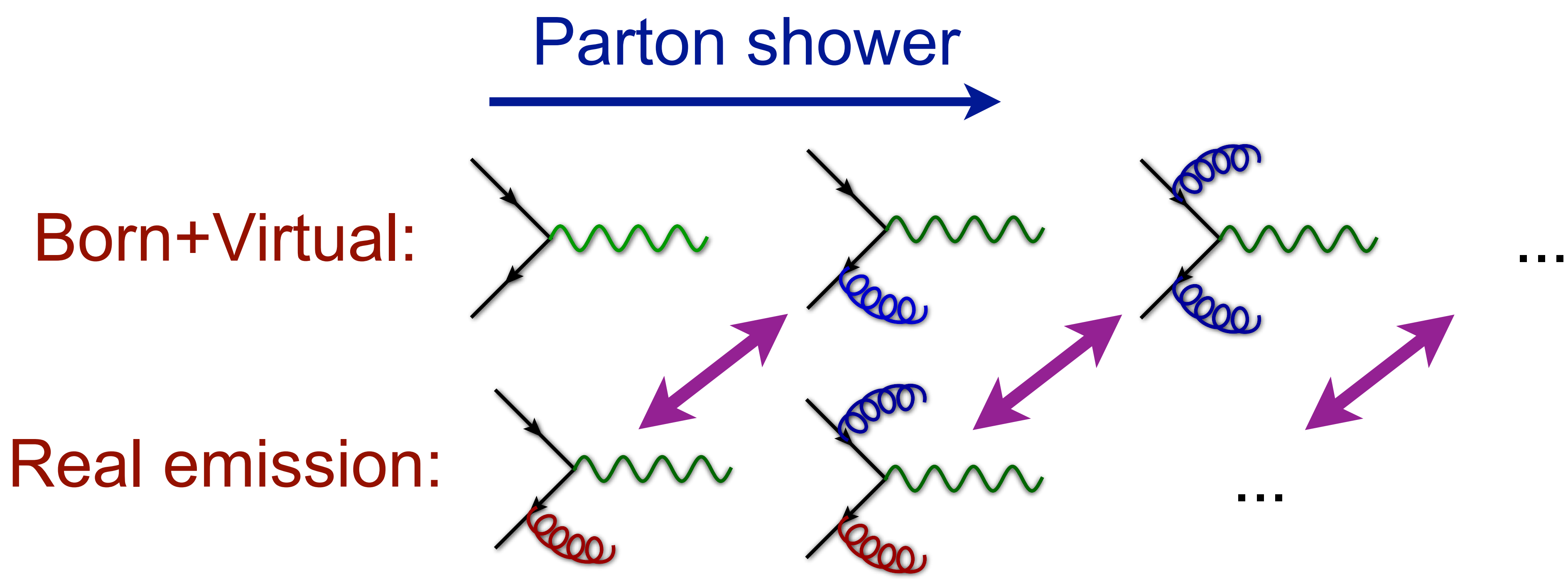
- Schematically $I_{\rm MC}^{(k)}(O)$ for 0 and 1 emission is given by

$$I_{\rm MC}^{(k)}(O) \sim \Delta_a(Q^2, Q_0^2) + \Delta_a(Q^2, t) \sum_{bc} dz \frac{dt}{t} \frac{d\phi}{2\pi} \frac{\alpha_s(t)}{2\pi} P_{a\to bc}(z)$$

- And Δ is the Sudakov factor

$$\Delta_a(Q^2, t) = \exp\left[-\sum_{bc} \int_t^{Q^2} \frac{dt'}{t'} dz \frac{d\phi}{2\pi} \frac{\alpha_s(t')}{2\pi} P_{a\to bc}\right]$$

Double counting



- There is double counting between the real emission matrix elements and the parton shower: the extra radiation can come from the matrix elements or the parton shower
- There is also an overlap between the virtual corrections and the Sudakov suppression in the zero-emission probability

Double counting in virtual/Sudakov

- The Sudakov factor Δ (which is responsible for the resummation of all the radiation in the shower) is the no-emission probability
- It's defined to be $\Delta = 1 - P$, where P is the probability for a branching to occur
- By using this conservation of probability in this way, Δ contains contributions from the virtual corrections implicitly
- Because at NLO the virtual corrections are already included via explicit matrix elements, Δ is double counting with the virtual corrections
- In fact, because the shower is unitary, what we are double counting in the real emission corrections is exactly equal to what we are double counting in the virtual corrections (but with opposite sign)!

Avoiding double counting

- There are a couple of methods to circumvent this double counting
  - **MC@NLO** (Frixione & Webber)
  - **POWHEG** (Nason)
  - KRKNLO (Cracow group), Vincia (Skands et al.), Geneva (Alioli et al.), …

MC@NLO procedure

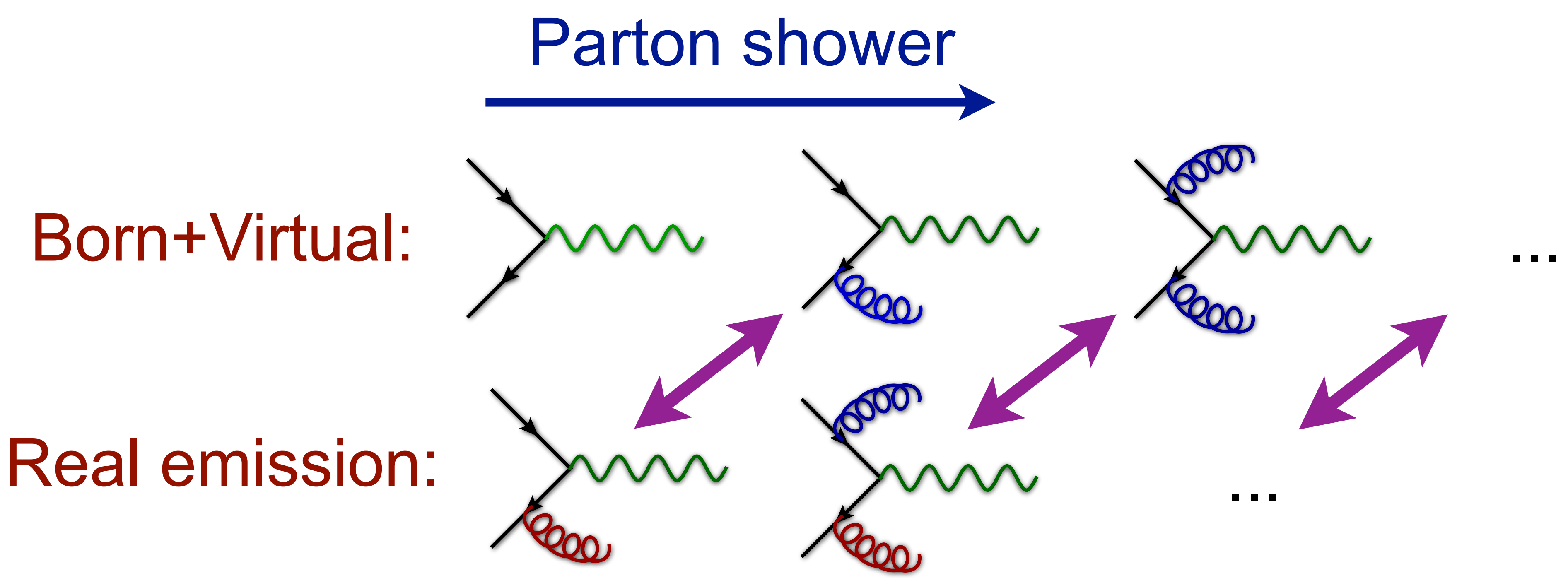
Frixione & Webber (2002)

- To remove the double counting, we can add and subtract the same term to the *m* and *m*+1 body configurations

$$\frac{d\sigma_{\mathrm{MC@NLO}}}{dO} = \left[d\Phi_m (B + \int_{\mathrm{loop}} V + \int d\Phi_1 MC) \right] I_{\mathrm{MC}}^{(m)}(O) + \left[d\Phi_{m+1} (R - MC) \right]) I_{\mathrm{MC}}^{(m+1)}(O)$$

Where the *MC* are defined to be the contribution of the parton shower to get from the *m* body Born final state to the *m*+1 body real emission final state

MC@NLO procedure



- Double counting is explicitly removed by including the “shower subtraction terms”

$$\frac{d\sigma_{\mathrm{MC@NLO}}}{dO} = \left[d\Phi_m \left(B + \int_{\mathrm{loop}} V + \int d\Phi_1 MC\right)\right] I_{\mathrm{MC}}^{(m)}(O)$$
$$+ \left[d\Phi_{m+1}(R - MC) \right]) I_{\mathrm{MC}}^{(m+1)}(O)$$

MC@NLO properties

- Good features of including the subtraction counter terms
  1. **Double counting avoided**: The rate expanded at NLO coincides with the total NLO cross section
  2. **Smooth matching**: MC@NLO coincides (in shape) with the parton shower in the soft/collinear region, while it agrees with the NLO in the hard region
  3. **Stability**: weights associated to different multiplicities are separately finite. The *MC* term has the same infrared behavior as the real emission (there is a subtlety for the soft divergence)
- Not so nice feature:
  4. **Parton shower dependence**: the form of the *MC* terms depends on what the parton shower does exactly. Need special subtraction terms for each parton shower to which we want to match: updates in showers might not be compatible with *MC* terms

Double counting avoided

$$\frac{d\sigma_{\mathrm{MC@NLO}}}{dO} = \left[d\Phi_m(B + \int_{\mathrm{loop}} V + \int d\Phi_1 MC)\right] I_{\mathrm{MC}}^{(m)}(O) + \left[d\Phi_{m+1}(R - MC)\right])I_{\mathrm{MC}}^{(m+1)}(O)$$

- Expanded at NLO

$$I_{\mathrm{MC}}^{(m)}(O)dO = 1 - \int d\Phi_1 \frac{MC}{B} + d\Phi_1 \frac{MC}{B} + \ldots$$

$$d\sigma_{\mathrm{NLOwPS}} = \left[d\Phi_m(B + \int_{\mathrm{loop}} V + \int d\Phi_1 MC)\right] I_{\mathrm{MC}}^{(m)}(O)dO + \left[d\Phi_{m+1}(R - MC)\right] \simeq d\Phi_m(B + \int_{\mathrm{loop}} V) + d\Phi_{m+1}R = d\sigma_{\mathrm{NLO}}$$

Smooth matching

$$\frac{d\sigma_{\mathrm{MC@NLO}}}{dO} = \left[d\Phi_m(B + \int_{\mathrm{loop}} V + \int d\Phi_1 MC)\right] I_{\mathrm{MC}}^{(m)}(O)$$
$$+ \left[d\Phi_{m+1}(R - MC)\right])I_{\mathrm{MC}}^{(m+1)}(O)$$

- Smooth matching:
  - Soft/collinear region: $R \simeq MC \quad \Rightarrow \; d\sigma_{\mathrm{MC@NLO}} \sim I_{\mathrm{MC}}^{(m)}(O)dO$
  - Hard region (shower effects suppressed), ie.

$$MC \simeq 0 \qquad I_{\mathrm{MC}}^{(m)}(O) \simeq 0 \qquad I_{\mathrm{MC}}^{(m+1)}(O) \simeq 1$$
$$\Rightarrow d\sigma_{\mathrm{MC@NLO}} \sim d\Phi_{m+1} R$$

Stability & unweighting

$$\frac{d\sigma_{\text{MC@NLO}}}{dO} = \left[d\Phi_m\left(B + \int_{\text{loop}} V + \int d\Phi_1 MC\right)\right] I_{\text{MC}}^{(m)}(O)$$
$$+ \left[d\Phi_{m+1}(R - MC)\right])I_{\text{MC}}^{(m+1)}(O)$$

- The *MC* subtraction terms are defined to be what the shower does to get from the *m* to the *m*+1 body matrix elements. Therefore the cancellation of singularities is exact in the (*R* - *MC*) term*: there is no mapping of the phase-space in going from events to counter events as we have in the CS-dipoles/FKS subtraction
- The integral is bounded all over phase-space; we can therefore generate **unweighted events**!
  - "S-events" (which have *m* body kinematics)
  - "H-events" (which have *m*+1 body kinematics)

* up to a subtlety related to the soft limit and gluon helicity dependence

Negative weights

$$\frac{d\sigma_{\text{MC@NLO}}}{dO} = \left[d\Phi_m\left(B + \int_{\text{loop}} V + \int d\Phi_1 MC\right)\right] I_{\text{MC}}^{(m)}(O)$$
$$+ \left[d\Phi_{m+1}(R - MC)\right]) I_{\text{MC}}^{(m+1)}(O)$$

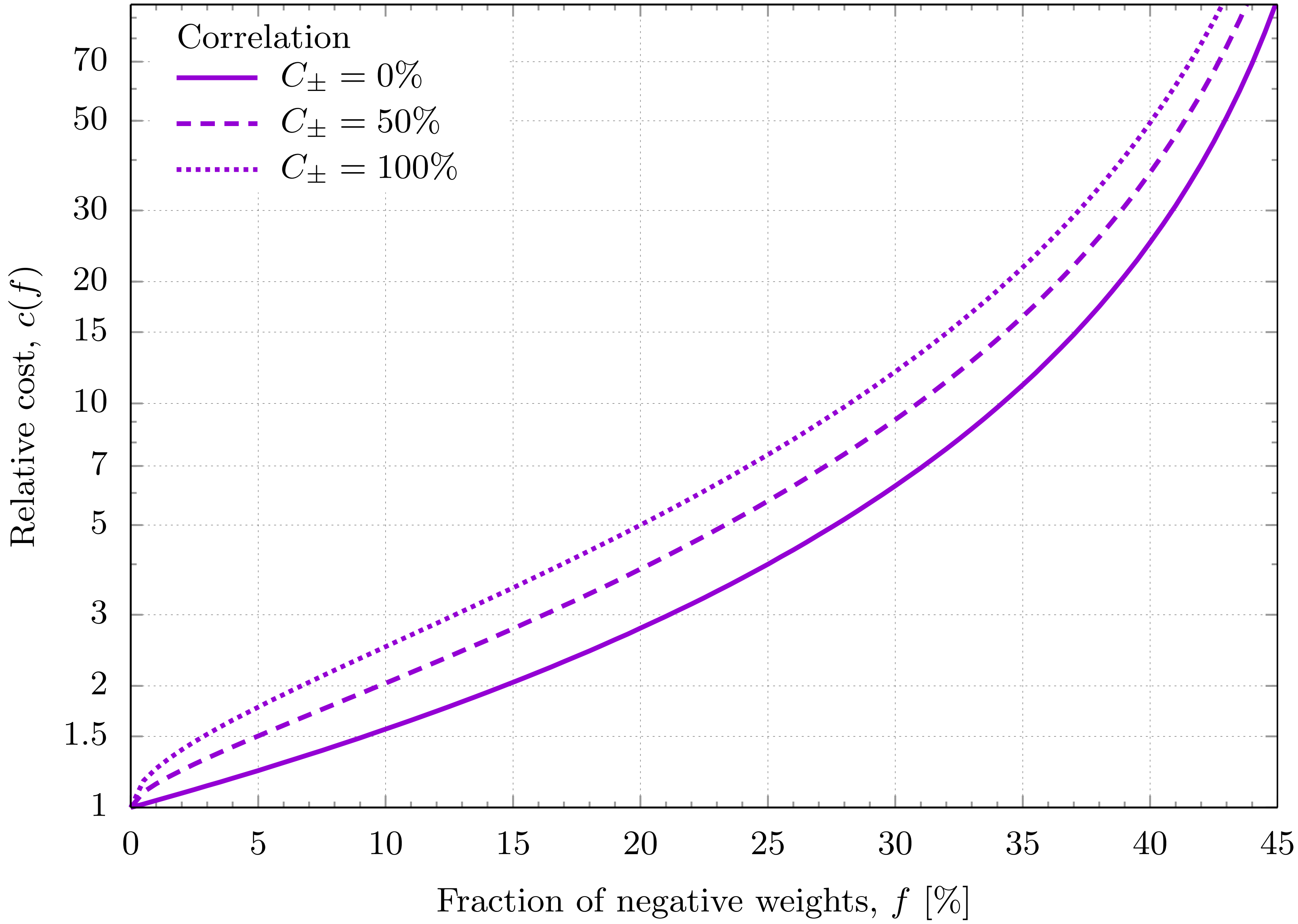
- We generate events for the two terms between the square brackets (S- and H-events) separately
- There is no guarantee that these contributions are separately positive (even though predictions for infra-red safe observables should always be positive!)
- Therefore, when we do event unweighting we can only unweight the events **up to a sign**. These signs should be taken into account when doing a physics analysis
- The events are only physical when they are showered

Possible issues with the MC@NLO method

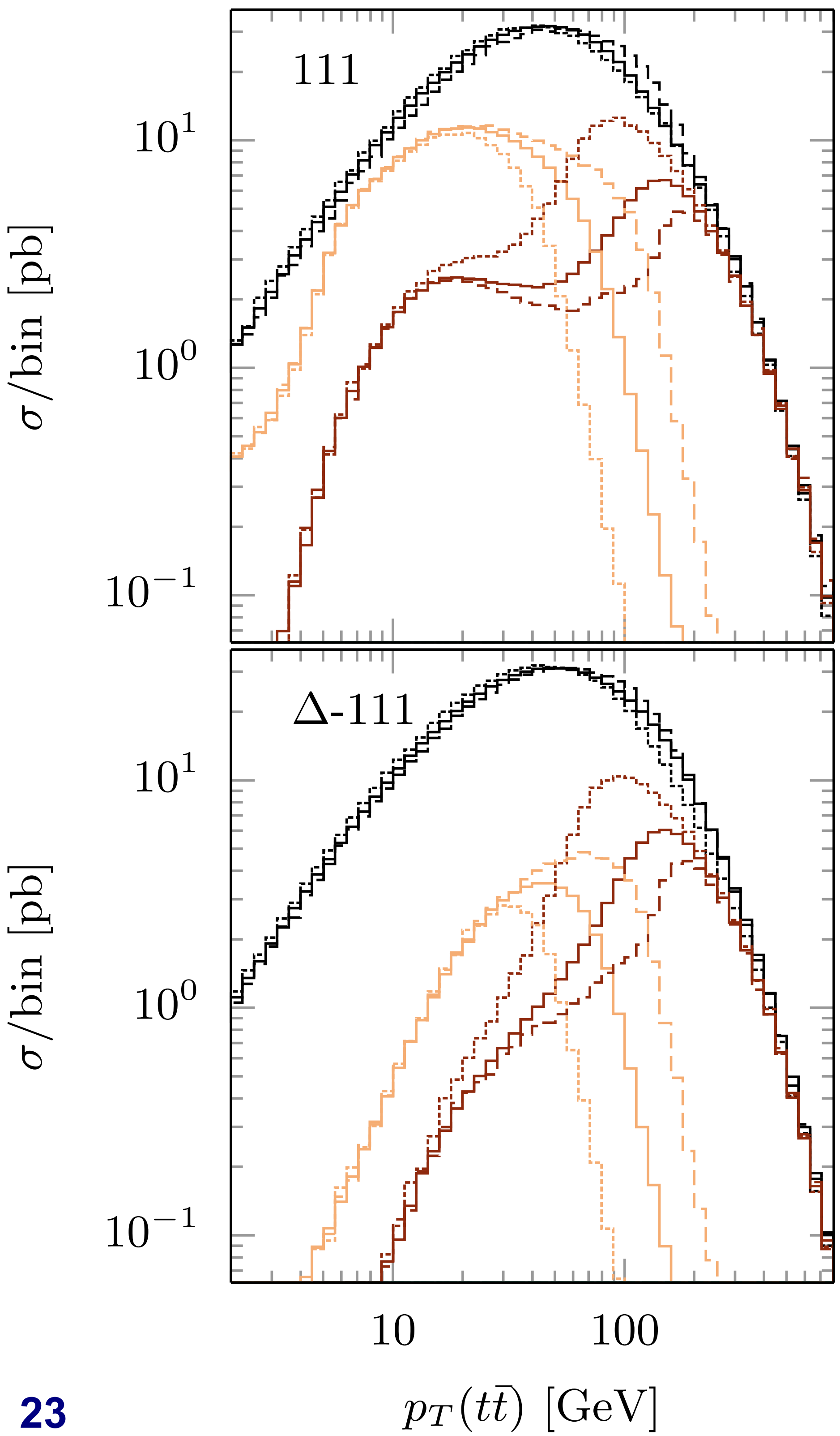
- MC subtraction terms need to be defined over the full phase-space, even though the shower has a cut-off.
  - Can be considered a power corrections to the parton shower and is therefore beyond expected accuracy
- Value of the scale entering α_S in the MC subtraction terms
  - Can be considered a higher order difference and is therefore beyond expected accuracy
- Shower does, in general, not reproduce exactly the IR singularities in the soft limit (for subleading terms in colour)
  - Can be considered a power corrections and is therefore beyond expected accuracy
  - Other solution would be to change the shower to include complete colour dependence (at least for a single emission)
- **Fraction of negative weights can be large**
  (20-30% negative weights is not uncommon)
  - Requires larger samples of unweighted events to obtain the same statistical precision

Cost of negative weights

- The computational costs to generate events negative weights can be enormous: for physical observables they cancel against positive weight events, but the overall sample still carries the statistical uncertainty of the full sample:



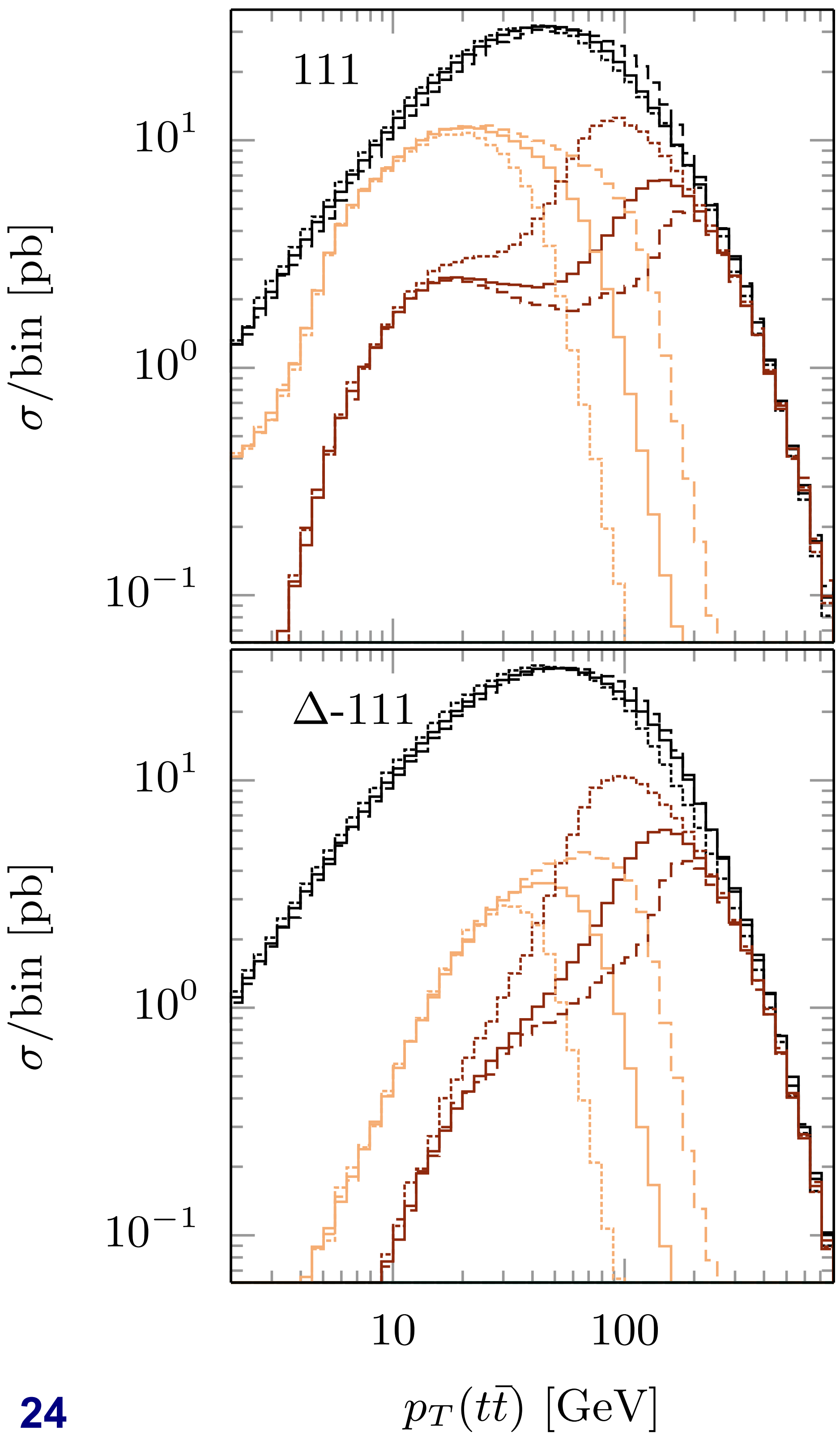
MC@NLO-Δ



- Top pair production
- After shower: black
- Before shower, H-events:
  - with negative weights: light brown
  - with positive weights: dark drown
- Negative weights dominate at small pT:
  - even though difference between MC term and R is finite, it is not necessarily small and/or positive

MC@NLO-Δ

RF, Frixione, Prestel, Torrielli (2020)



- Since the bulk of the negative weights is at small transverse momentum, the (shape of the) observable is dominated by showering the S-events

$$d\sigma^{(\Delta,\mathbb{H})} = \left(d\sigma^{(\mathrm{NLO},E)} - d\sigma^{(\mathrm{MC})}\right)\Delta\,,$$

$$d\sigma^{(\Delta,\mathbb{S})} = d\sigma^{(\mathrm{MC})}\Delta + \sum_{\alpha=S,C,SC} d\sigma^{(\mathrm{NLO},\alpha)} + d\sigma^{(\mathrm{NLO},E)}\left(1-\Delta\right)$$

- Hence, we should be able to damp this region, and add the difference to the S-events!

MC@NLO-Δ

RF, Frixione, Prestel, Torrielli (2020)

	MC@NLO			MC@NLO-Δ		
	111	221	441	Δ-111	Δ-221	Δ-441
$pp \to e^+e^-$	6.9% (1.3)	3.5% (1.2)	3.2% (1.1)	5.7% (1.3)	2.4% (1.1)	2.0% (1.1)
$pp \to e^+\nu_e$	7.2% (1.4)	3.8% (1.2)	3.4% (1.2)	5.9% (1.3)	2.5% (1.1)	2.3% (1.1)
$pp \to H$	10.4% (1.6)	4.9% (1.2)	3.4% (1.2)	7.5% (1.4)	2.0% (1.1)	0.5% (1.0)
$pp \to Hb\bar{b}$	40.3% (27)	38.4% (19)	38.0% (17)	36.6% (14)	32.6% (8.2)	31.3% (7.2)
$pp \to W^+j$	21.7% (3.1)	16.5% (2.2)	15.7% (2.1)	14.2% (2.0)	7.9% (1.4)	7.4% (1.4)
$pp \to W^+t\bar{t}$	16.2% (2.2)	15.2% (2.1)	15.1% (2.1)	13.2% (1.8)	11.9% (1.7)	11.5% (1.7)
$pp \to t\bar{t}$	23.0% (3.4)	20.2% (2.8)	19.6% (2.7)	13.6% (1.9)	9.3% (1.5)	7.7% (1.4)

- Fraction of negative weight events greatly reduced

POWHEG

Nason (2004)

- Consider the probability of the first emission of a leg (inclusive over later emissions)

$$d\sigma = d\Phi_m \, B \left[\Delta(Q^2, Q_0^2) + \Delta(Q^2, t) d\Phi_{(+1)} \frac{MC}{B} \right]$$

- One could try to get NLO accuracy by replacing B with the NLO rate (integrated over the extra phase-space)

$$B \to B + V + \int d\Phi_{(+1)} \, R$$

- This naive definition is not correct: the radiation is still described only at leading logarithmic accuracy, which is not correct for hard emissions.

POWHEG

- This is double counting.
  To see this, expand the equation up to the first emission

$$d\Phi_m \left[B + V + \int d\Phi_1 R\right]\left[1 - \int \Phi_1 \frac{MC}{B} + d\Phi_1 \frac{MC}{B}\right]$$

  which is not equal to the NLO

- In order to avoid double counting, one should replace the definition of the Sudakov form factor with the following:

$$\Delta(Q^2, Q_0^2) = \exp\left[-\int_{Q_0^2}^{Q^2} d\Phi_1 \frac{MC}{B}\right] \to \tilde{\Delta}(Q^2, Q_0^2) = \exp\left[-\int_{Q_0^2}^{Q^2} d\Phi_1 \frac{R}{B}\right]$$

  corresponding to a modified differential branching probability

$$d\tilde{p} = d\Phi_{(+1)} R/B$$

- Therefore we find for the POWHEG differential cross section

$$d\sigma_{\text{powheg}} = d\Phi_m \left[B + V + \int d\Phi_1 R\right]\left[\Delta(Q^2, Q_0^2) + \Delta(Q^2, t) d\Phi_1 \frac{R}{B}\right]$$

Properties

$$d\sigma_{\text{powheg}} = d\Phi_m \left[B + V + \int d\Phi_1 R \right] \left[\Delta(Q^2, Q_0^2) + \Delta(Q^2, t) d\Phi_1 \frac{R}{B} \right]$$

- The term in the square brackets integrates to one (integrated over the extra parton phase-space between scales Q_0^2 and Q^2)
  (this can also be understood as unitarity of the shower below scale t)
  POWHEG cross section is normalised to the NLO

- Expand up to the first-emission level:

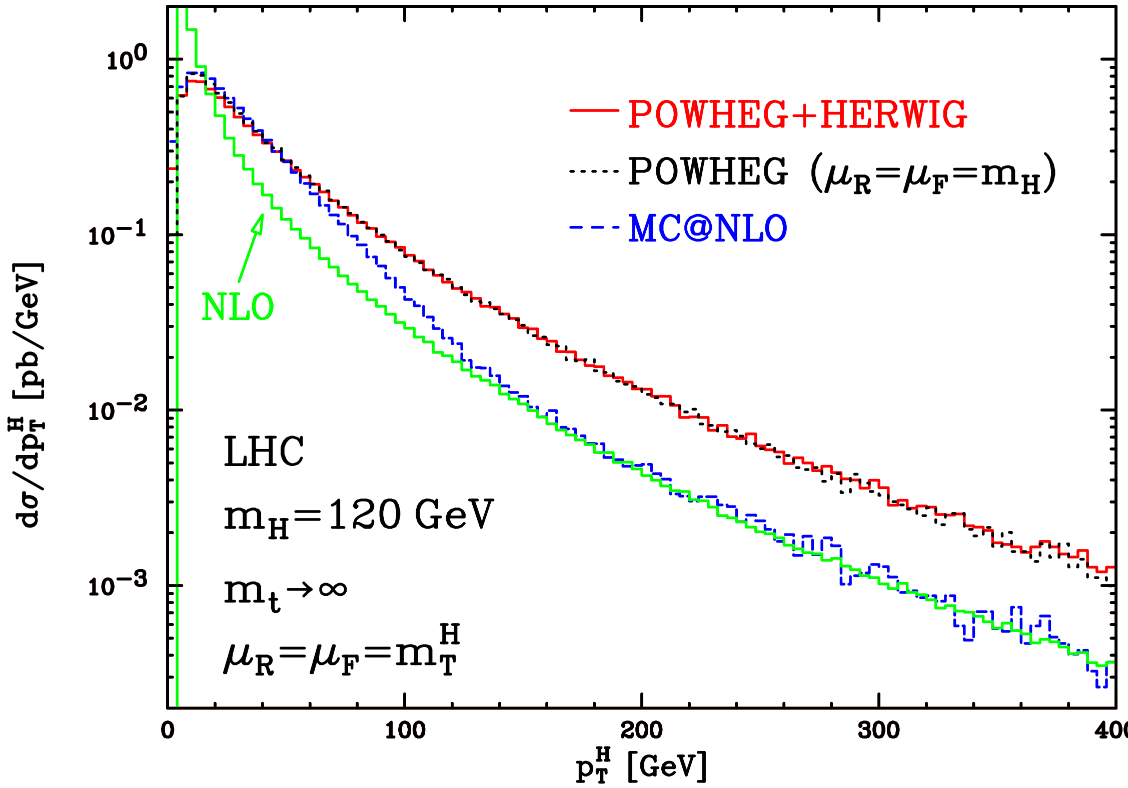
$$d\sigma_{\text{POWHEG}} = d\Phi_B \left[B + V + \int d\Phi_{(+1)} R \right] \left[1 - \int d\Phi_{(+1)} \frac{R}{B} + d\Phi_{(+1)} \frac{R}{B} \right] = d\sigma_{\text{NLO}}$$

  so double counting is avoided

- Its structure is identical an ordinary shower, with normalisation rescaled by a local K-factor and a different Sudakov for the first emission: no negative weights are involved.

Possible issues with POWHEG method

Higgs production in gluon fusion 0812.0578



- NLO-factor multiplies the complete first emission Sudakov terms: Large, arbitrary NNLO terms are included
  - scale dependence looks like NLO (i.e., is relatively small), even though distribution is only LO accurate in the tail
  - Can be ameliorated (see next slide)
- Order/evolution variable used in POWHEG and shower are not the same: formally needs a truncated, vetoed parton shower

$$d\sigma_{\rm POWHEG} = d\Phi_B \left[B + V + \int d\Phi_{(+1)} R\right] \left[\tilde{\Delta}(Q^2, Q_0^2) + \tilde{\Delta}(Q^2, t)\ d\Phi_{(+1)} \frac{R}{B}\right]$$

POWHEG: improved

In POWHEG, only singular part of real emission needs to be put in Sudakov:

$$d\sigma_{\mathrm{NLO+PS}} = d\Phi_B \bar{B}^s(\Phi_B)\left[\Delta^s(p_\perp^{\min}) + d\Phi_{R|B}\frac{R^s(\Phi_R)}{B(\Phi_B)}\Delta^s(p_T(\Phi))\right] + d\Phi_R R^f(\Phi_R)$$

where

$$\bar{B}^s(\Phi_B) = B(\Phi_B) + \left[V(\Phi_B) + \int d\Phi_{R|B} R^s(\Phi_{R|B})\right]$$

and we have split the Real emission matrix elements in a singular and finite part:

$$R(\Phi_R) = R^s(\Phi_R) + R^f(\Phi_R)$$

POWHEG: $R^s(\Phi) = F\, R(\Phi), \quad R^f(\Phi) = (1-F)R(\Phi)$

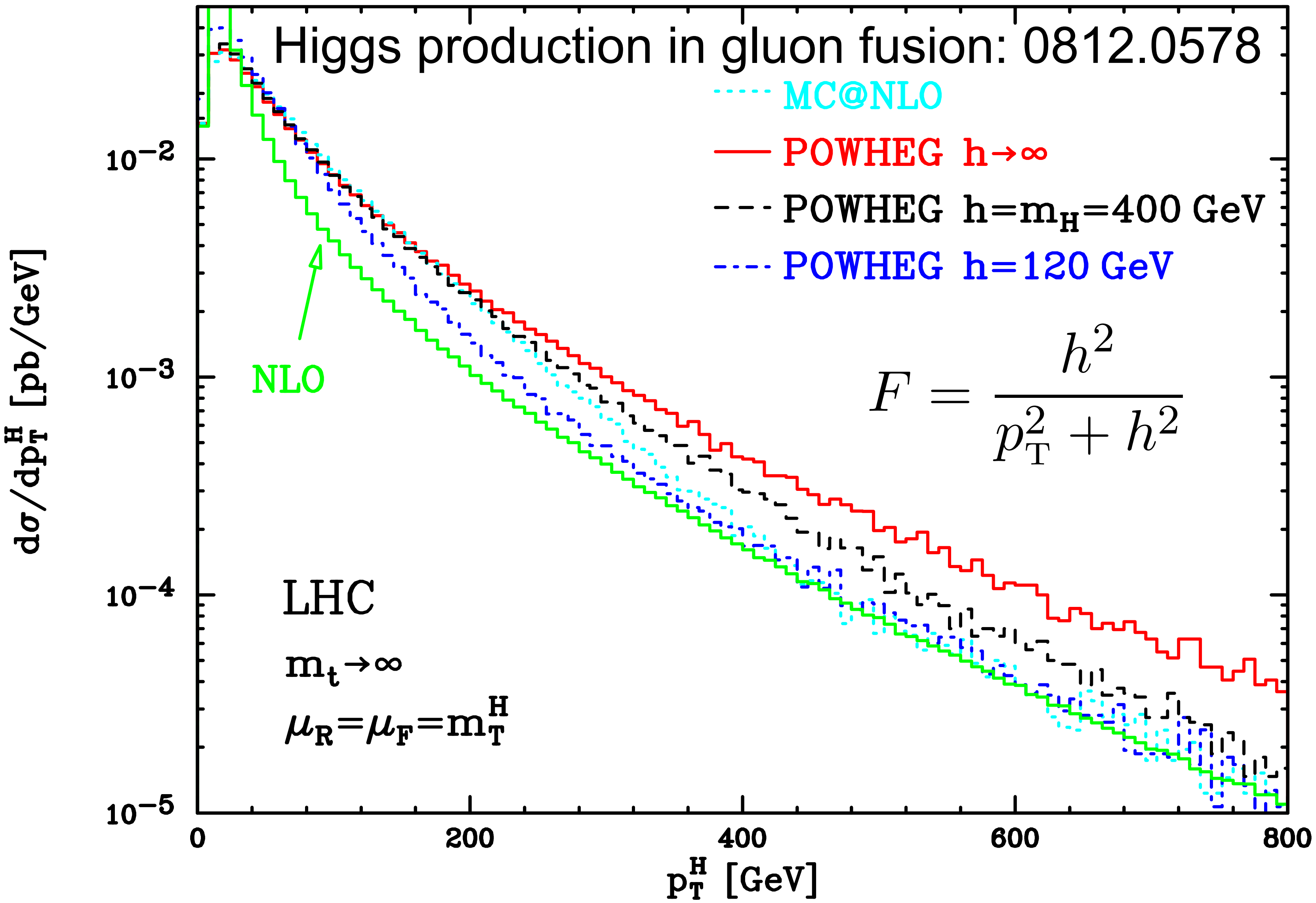
Original is $F = 1$: exponentiate the full real; it can be damped by hand

POWHEG looks now similar to MC@NLO.
MC@NLO has the real matrix elements split according to:

MC@NLO: $R^s(\Phi) = P(\Phi_{R|B})B(\Phi_B) = MC$

Need exact mapping $(\Phi_R, \Phi_B) \Rightarrow \Phi$ in MC subtraction term R^s

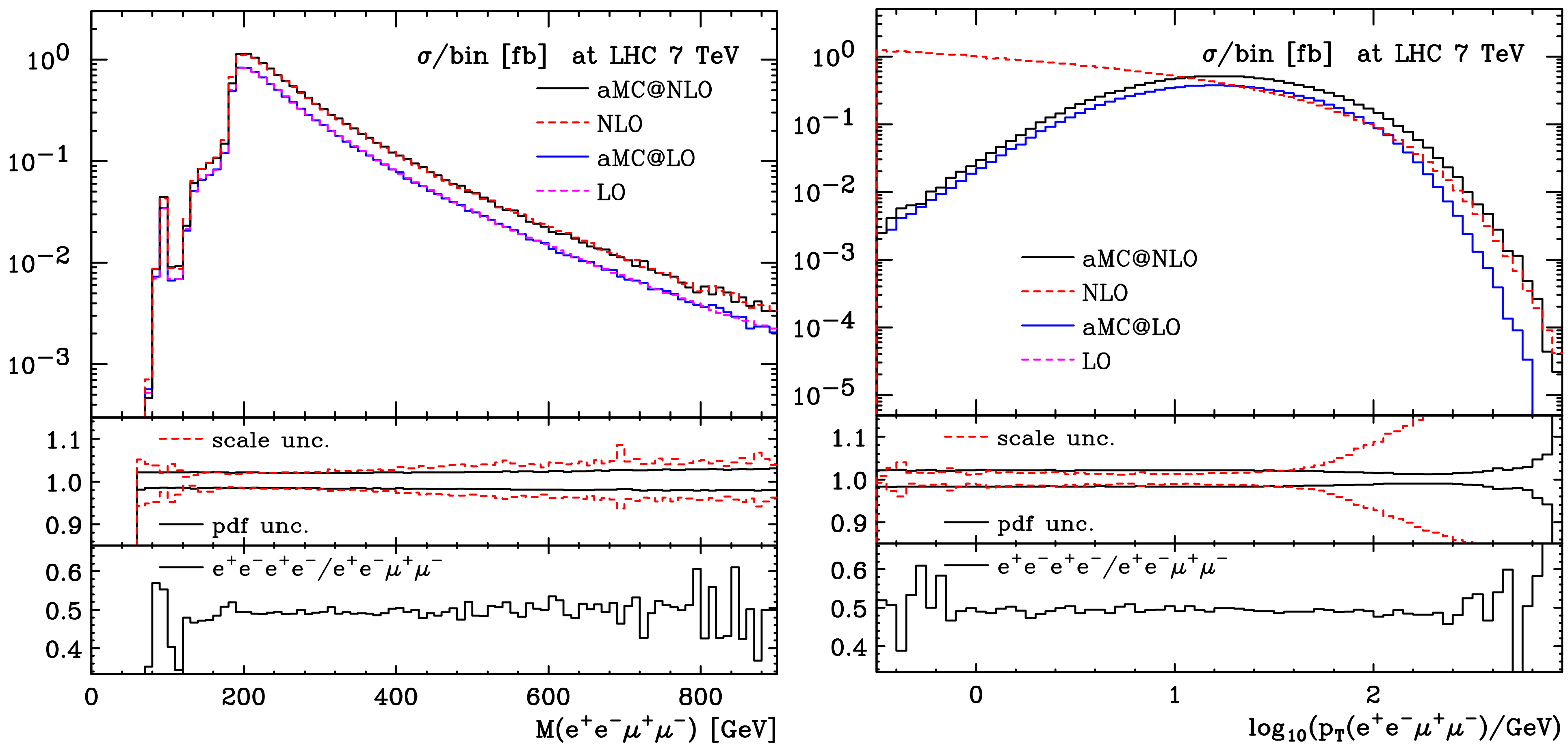
Damped powheg



- Inclusion of beyond-NLO terms can be varied by changing F
- Should this be considered an uncertainty or a tuning parameter?

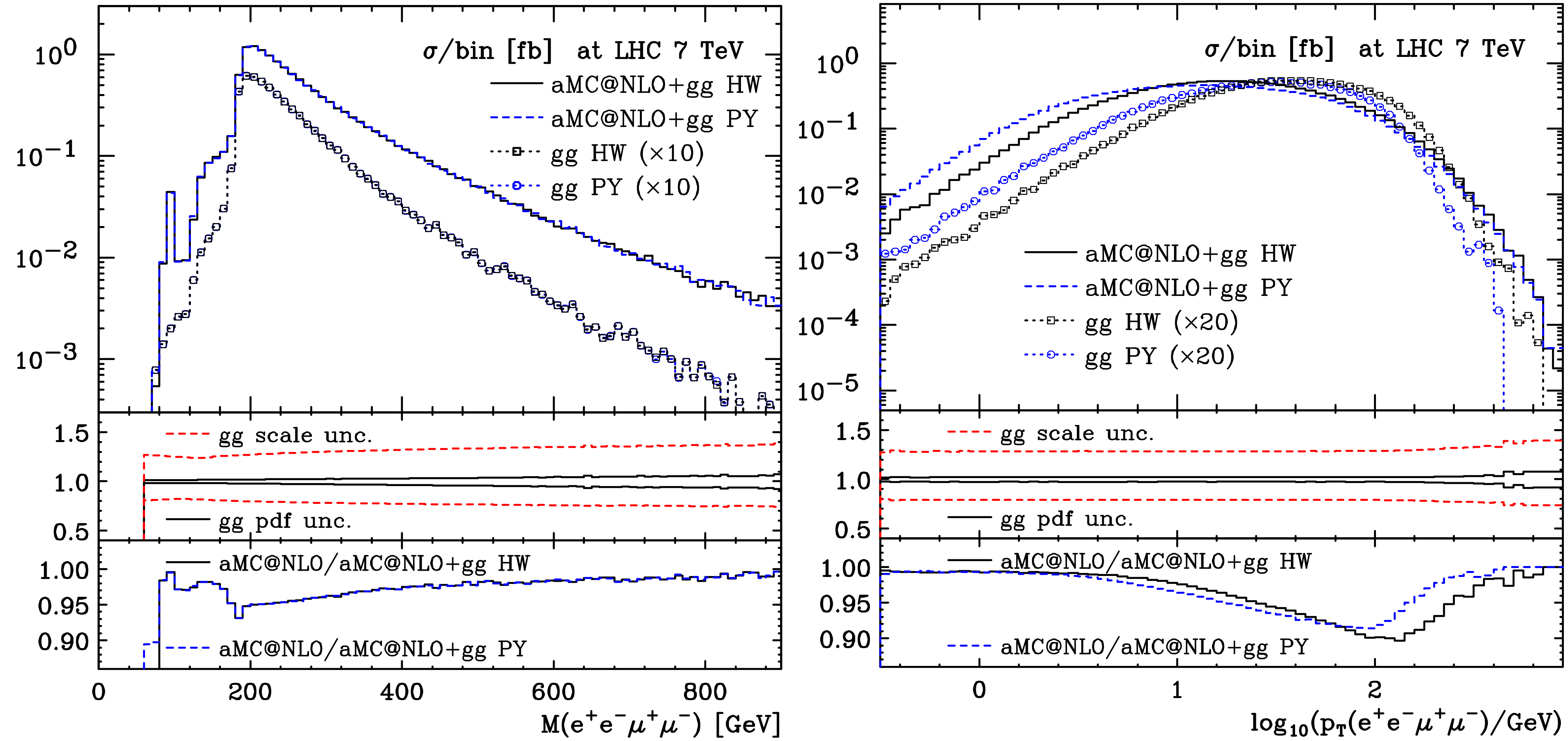
Four-lepton production

Plot from RF, Frixione, Hirschi, Maltoni, Pittau & Torrielli (2011)



- 4-lepton invariant mass is almost insensitive to parton shower effects. 4-lepton transverse moment is extremely sensitive

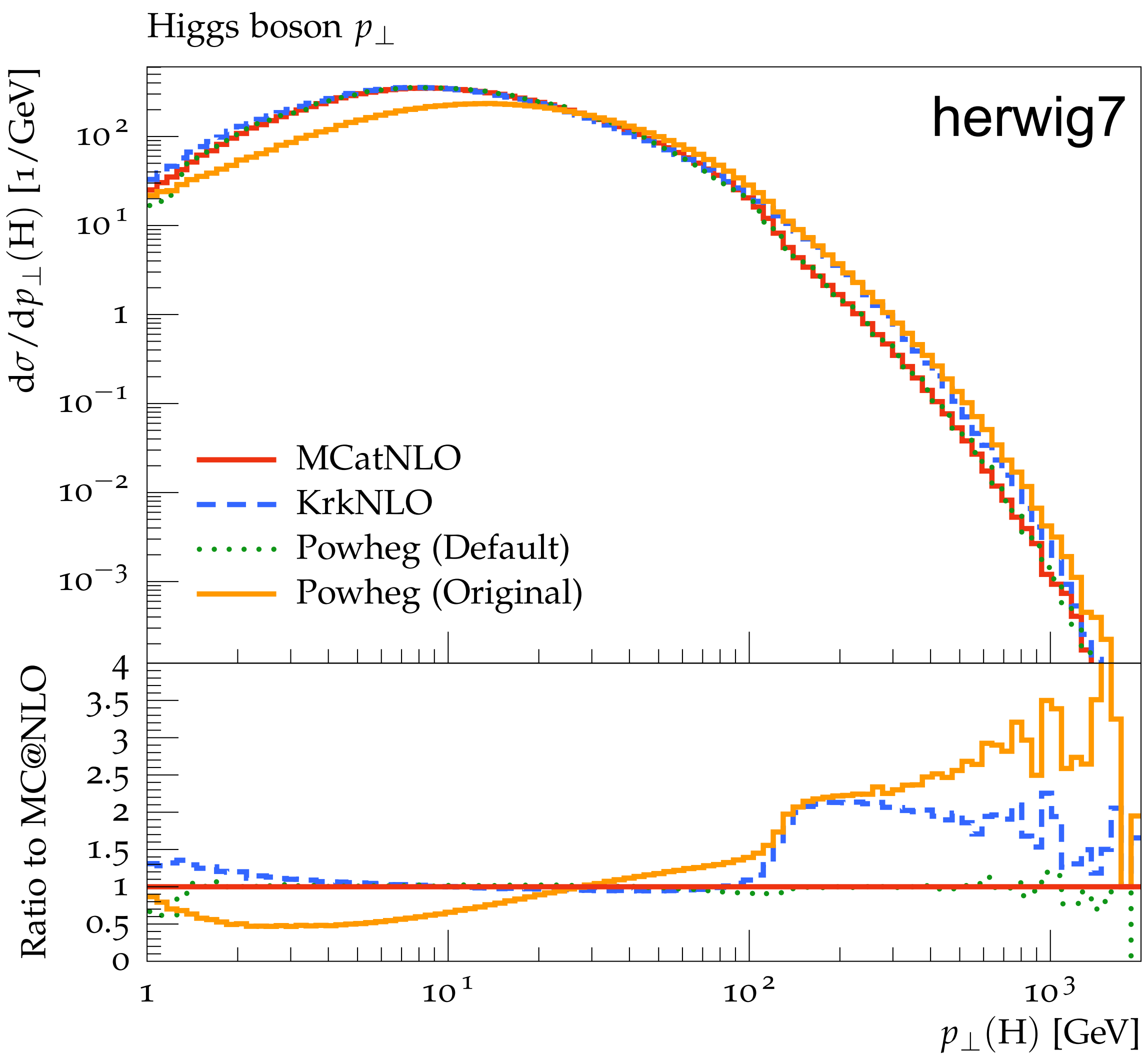
Four-lepton production

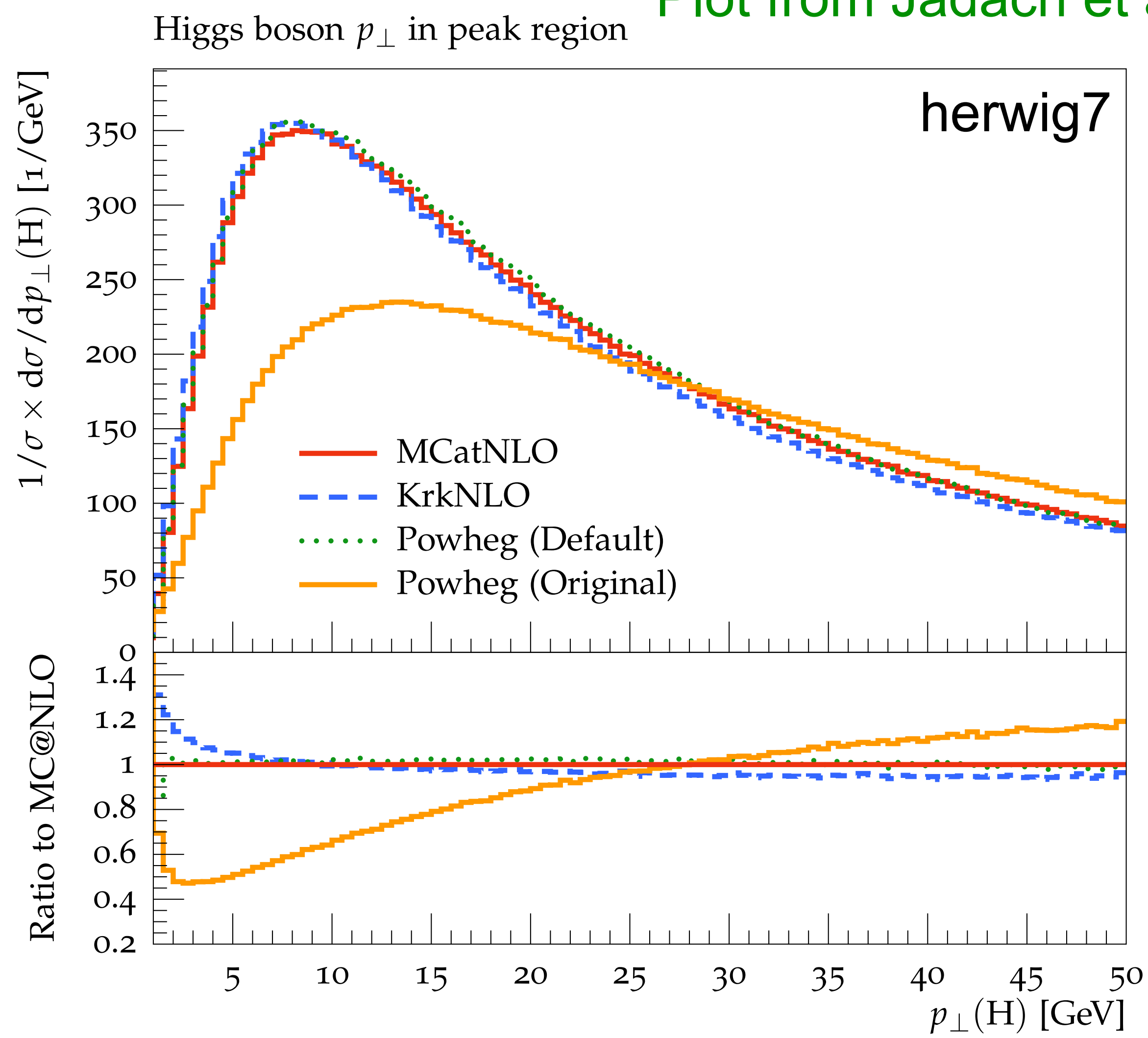


- Differences between Herwig (black) and Pythia (blue) showers large in the Sudakov suppressed region (much larger than the scale uncertainties)
- Contributions from gg initial state (formally NNLO) are of 5-10%

Higgs boson production

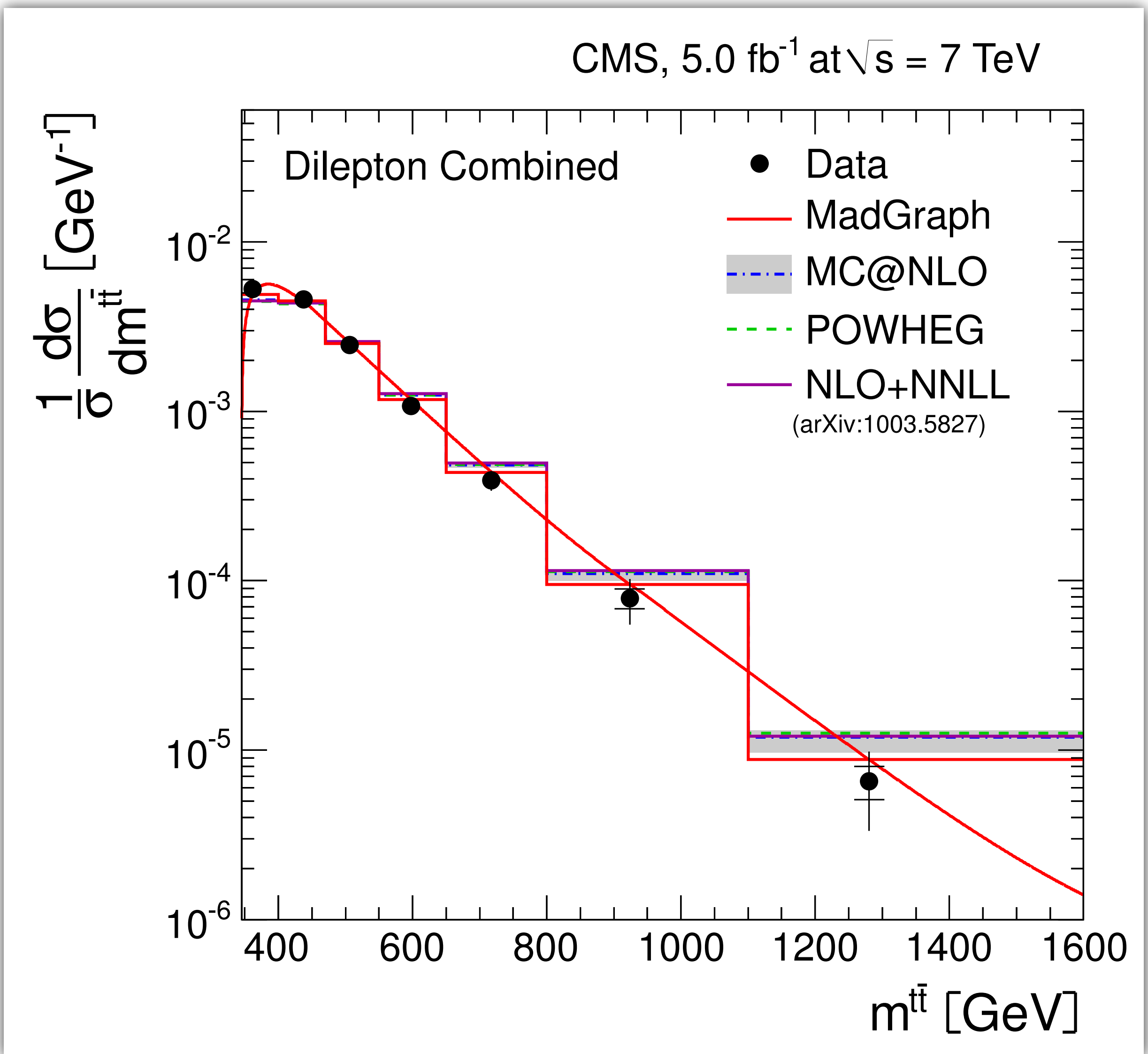
Plot from Jadach et al. (2016)

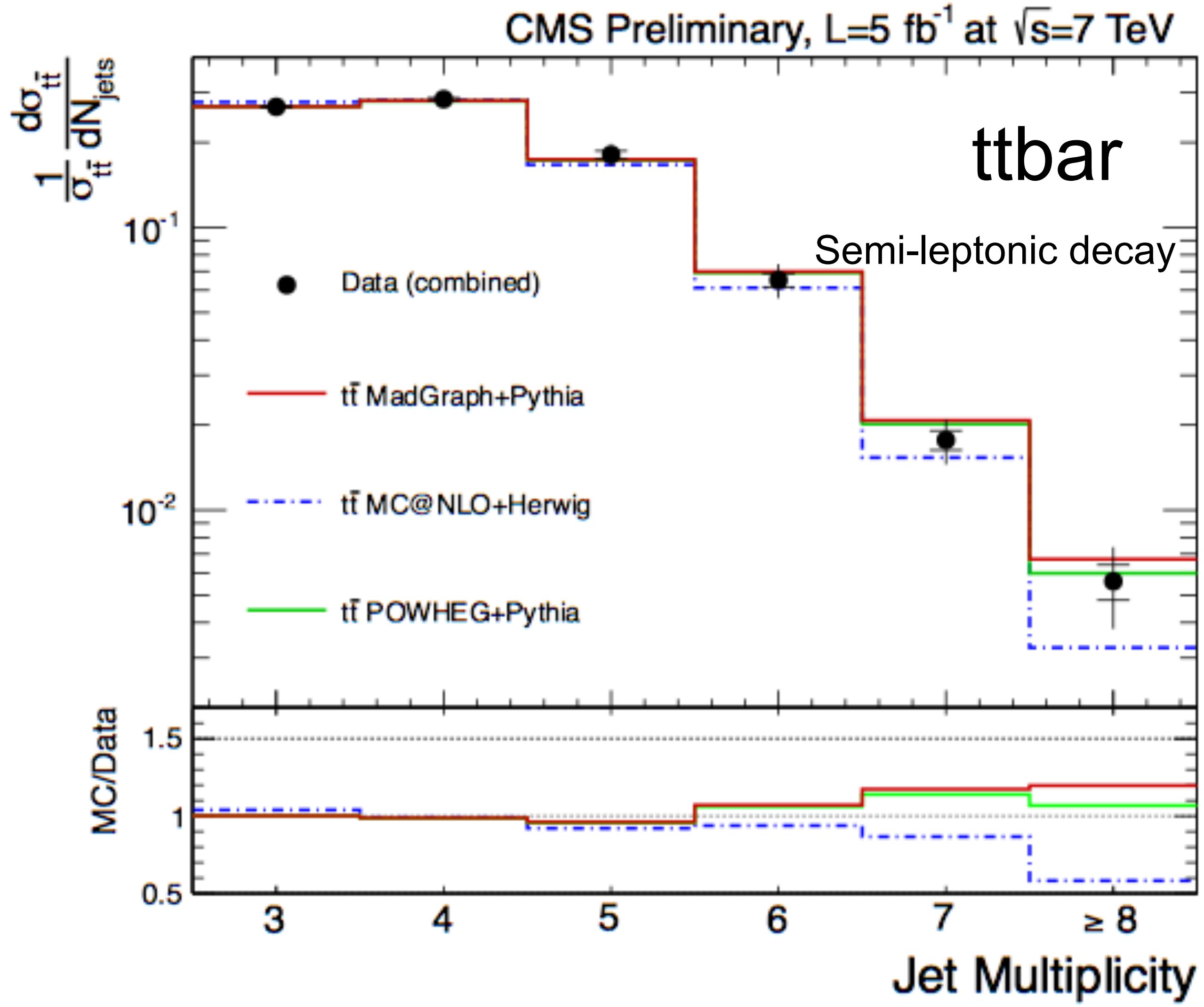




- Powheg: original: F=1,
  default F={1 for $p_T(H) < m_H$, 0 for $p_T(H) > m_H$}
- Not only an impact at large p_T, but also at small p_T. Higher order terms in shower are large, hence can easily be tuned.

Is NLO+PS always the preferred method?

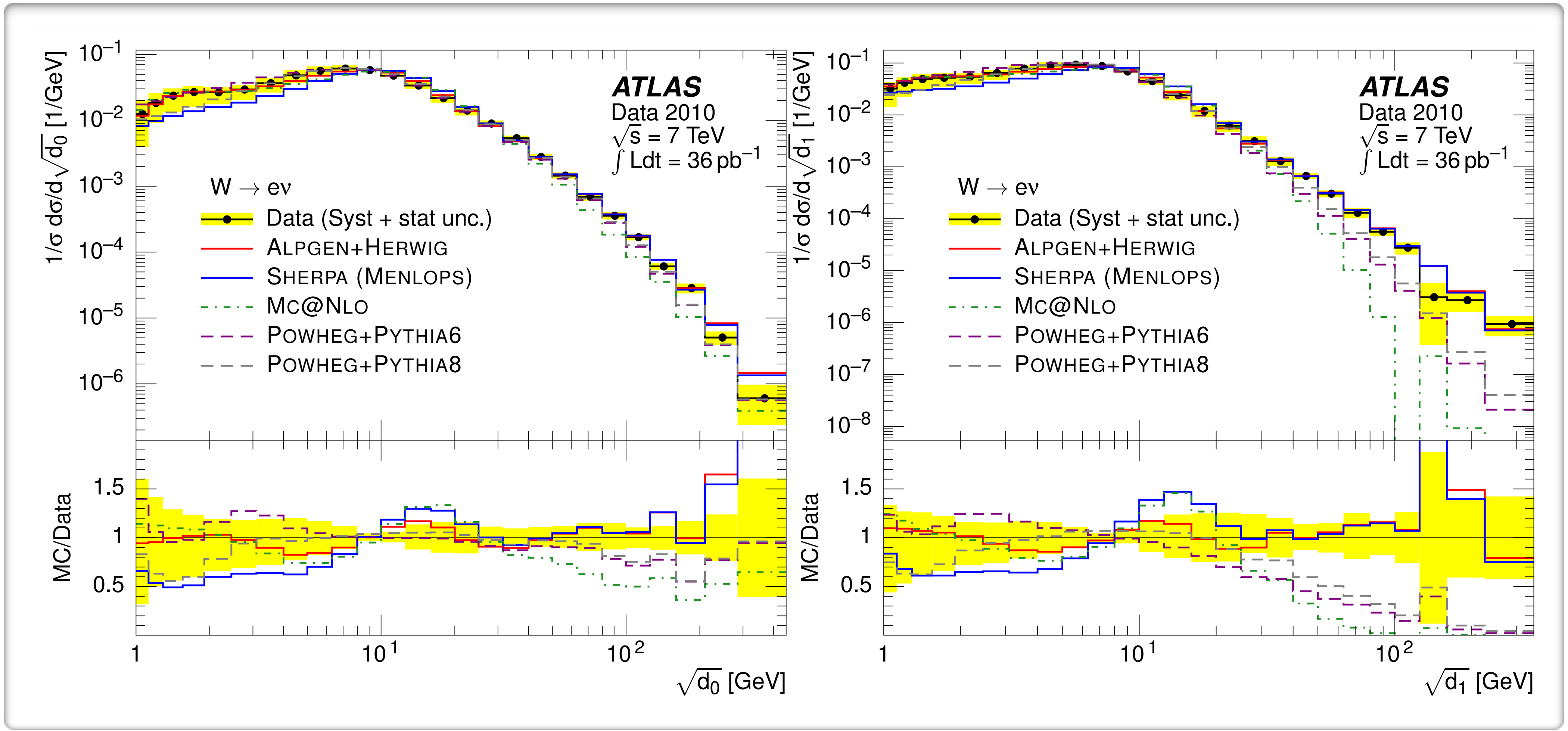




- It is the preferred method if the observable is described at NLO accuracy
- But there are many observables for which a given NLO+PS code has only zeroth order accuracy.

differential jet rates

1302.1415



- Effectively the scale for which a 1-jet event becomes a 0-jet event (left) or 2-jet event becomes a 1-jet event (based on k_T-algorithm)
- NLO+PS work well at low scales, but not so much at large scales: easily explained by only having LO (left) or PS (right) accuracy

Summary

- We want to match NLO computations to parton showers to keep the good features of both approximations
  - In the MC@NLO method:
    by including the shower subtraction terms in our process we avoid double counting between NLO processes and parton showers
  - In the POWHEG method:
    apply an NLO-factor, and modify the (Sudakov of the) first emission to fill the hard region of phase-space according to the real-emission matrix elements