Lectures on

Parton Shower matching at NLO

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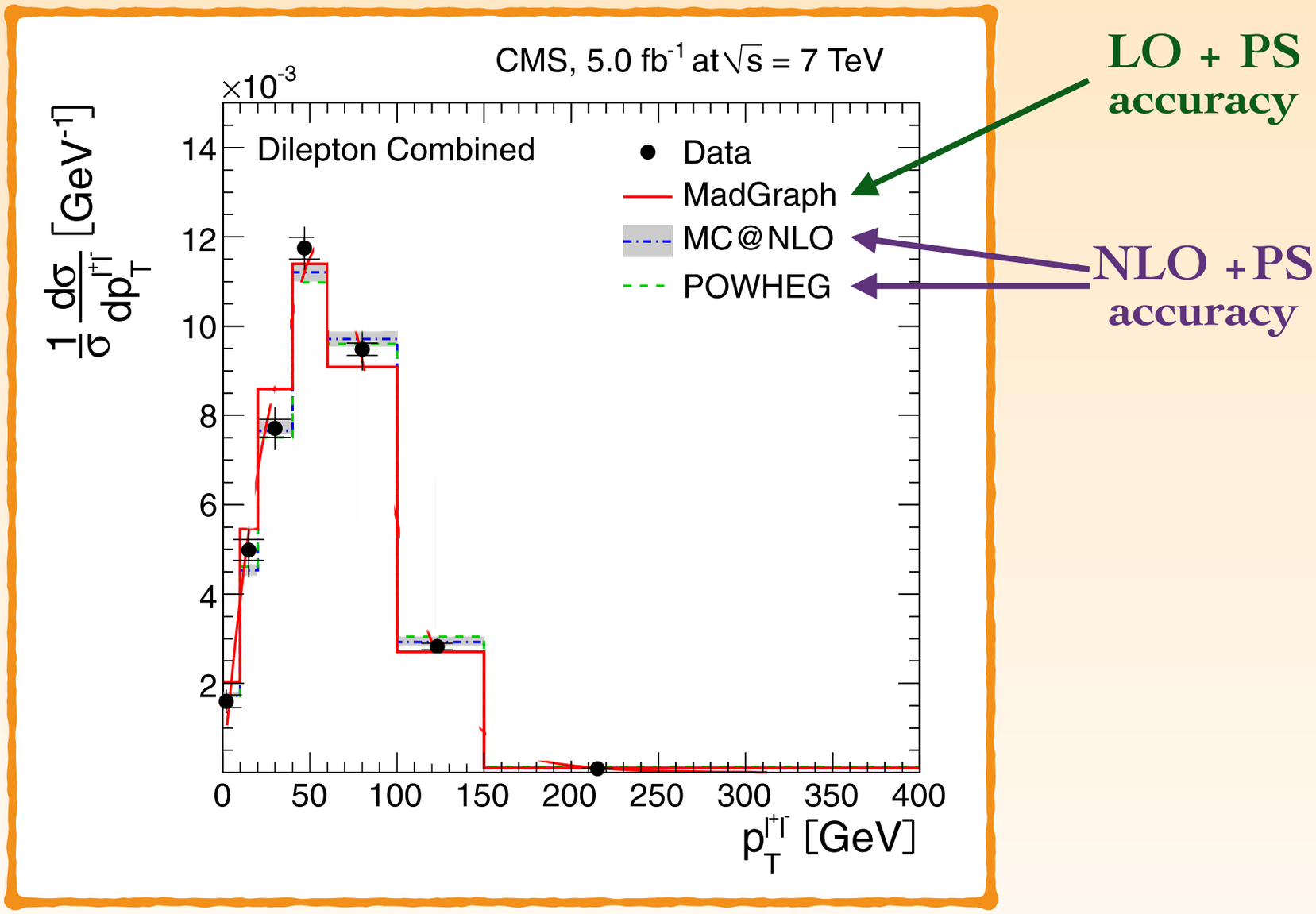
Parton showers and leading order predictions

- In Andrzej's lectures, he discussed in detail how parton showers work
- However
  - always started from a leading order hard process
  - all radiation (even very hard) is described by the shower
- This is suboptimal

Need for NLO

- NLO predictions improve over LO predictions in many 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 the formal accuracy of predictions

- 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
  - Combine the two above methods!

Matrix elements + parton shower merging at LO

Matrix elements vs. Parton showers

Matrix elements vs. Parton showers

ME

1. Fixed order calculation
2. Computationally expensive
3. Limited number of particles
4. Valid when partons are hard and well separated
5. Quantum interference correct
6. Needed for multi-jet description

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Shower MC

1. Resums logs to all orders
2. Computationally cheap
3. No limit on particle multiplicity
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Approaches are complementary: merge them!

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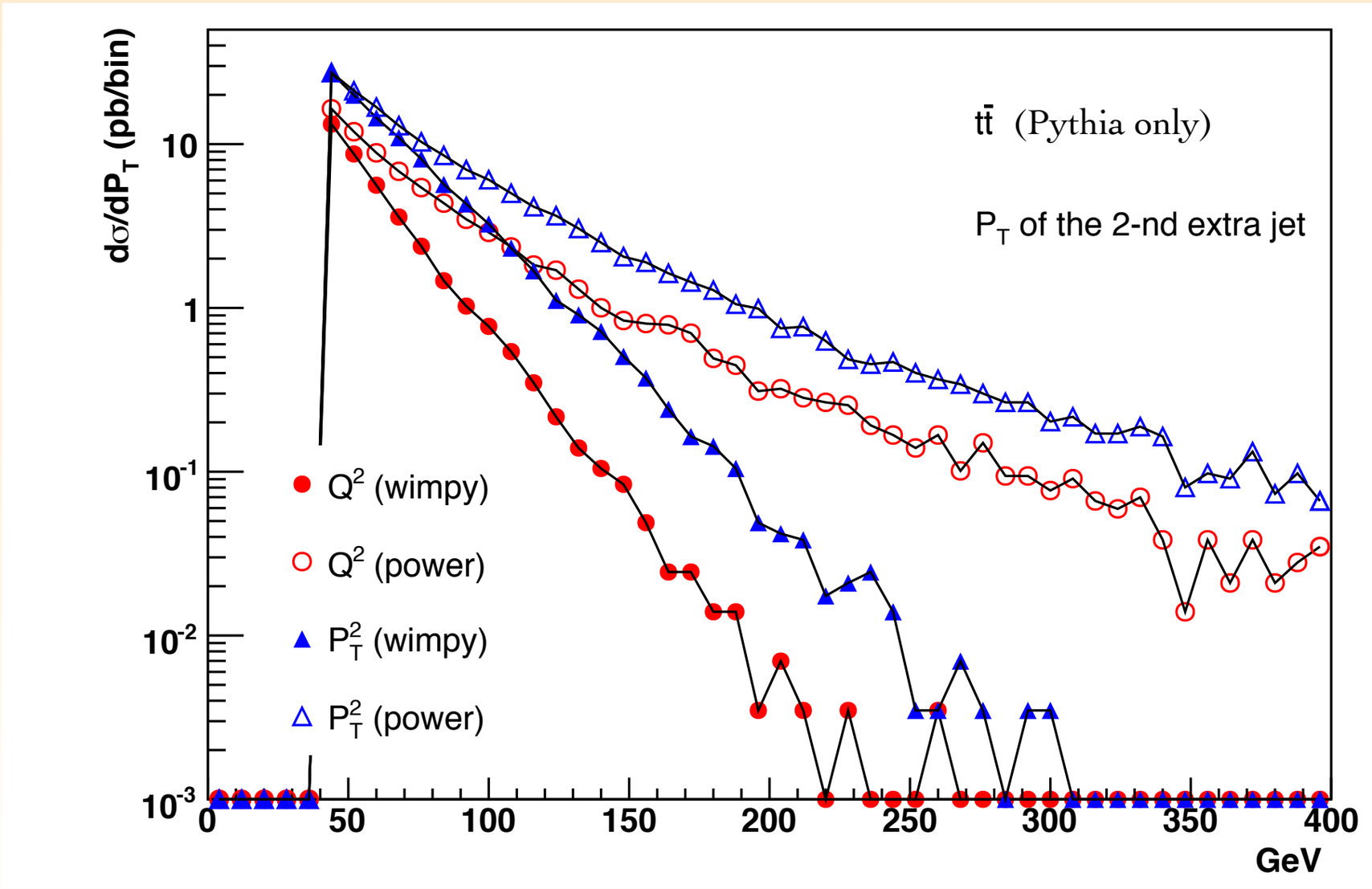
Approaches are complementary: merge them!

Difficulty: avoid double counting, ensure smooth distributions

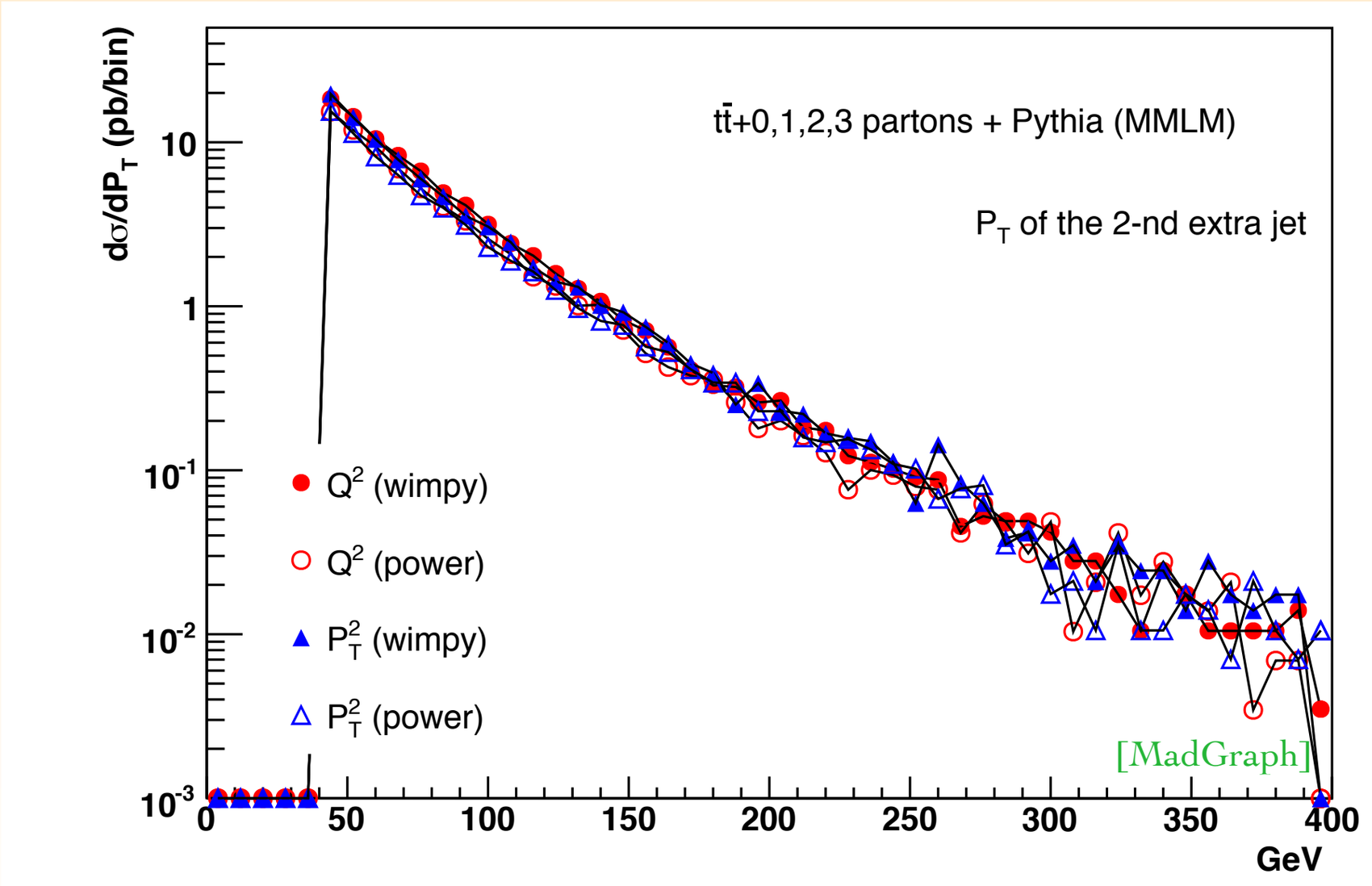
PS alone vs. Matched sample

In the soft-collinear approximation of Parton Shower MCs, parameters are used to tune the result ⇒ Large variation in results (small prediction power)



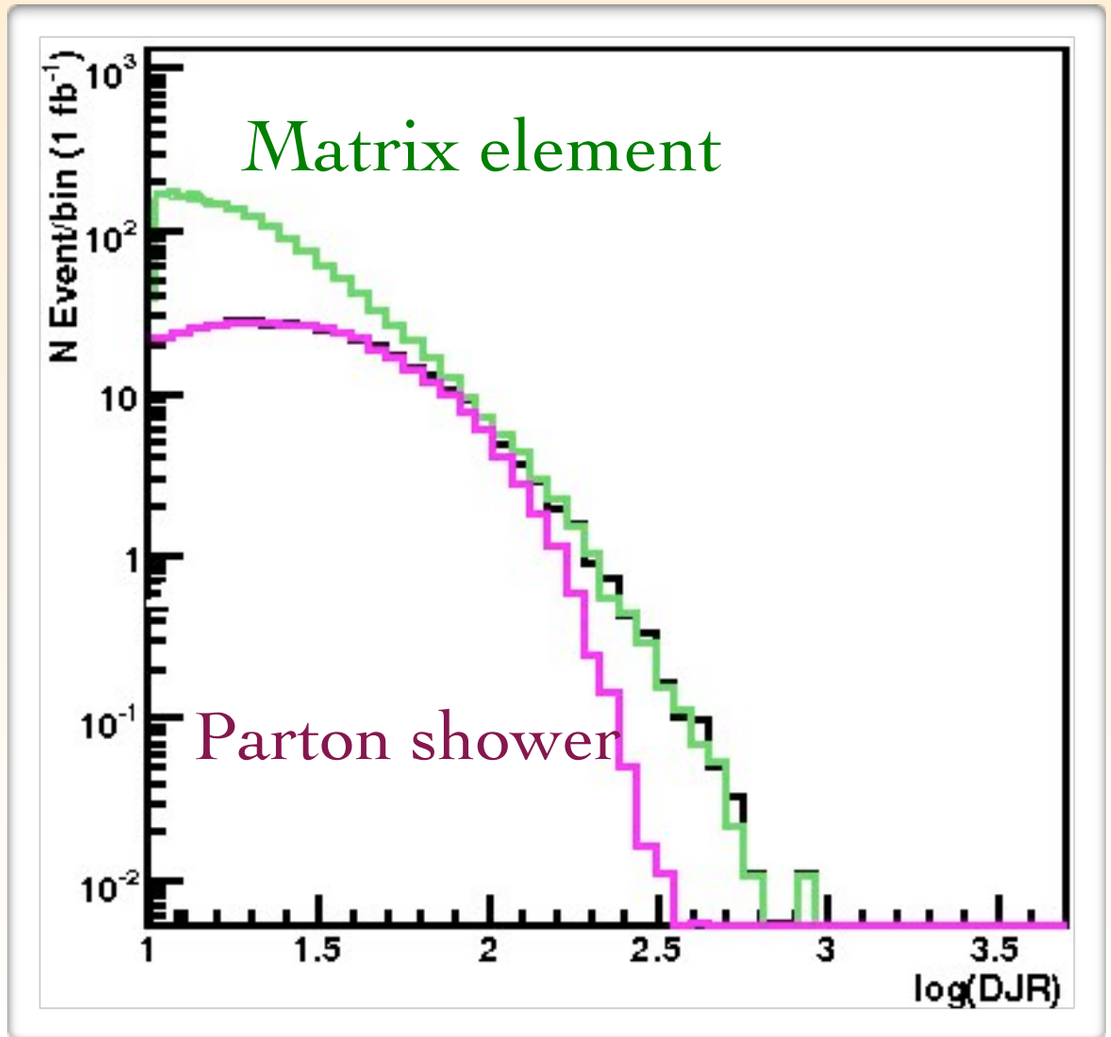
PS alone vs. Matched sample

In a matched sample these differences are irrelevant since the behavior at high pt is dominated by the matrix element.



Goal for ME-PS merging/ matching

- ✦ Regularization of matrix element divergence
- ✦ Correction of the parton shower for large momenta
- ✦ Smooth jet distributions



2nd QCD radiation jet in top pair production at the LHC

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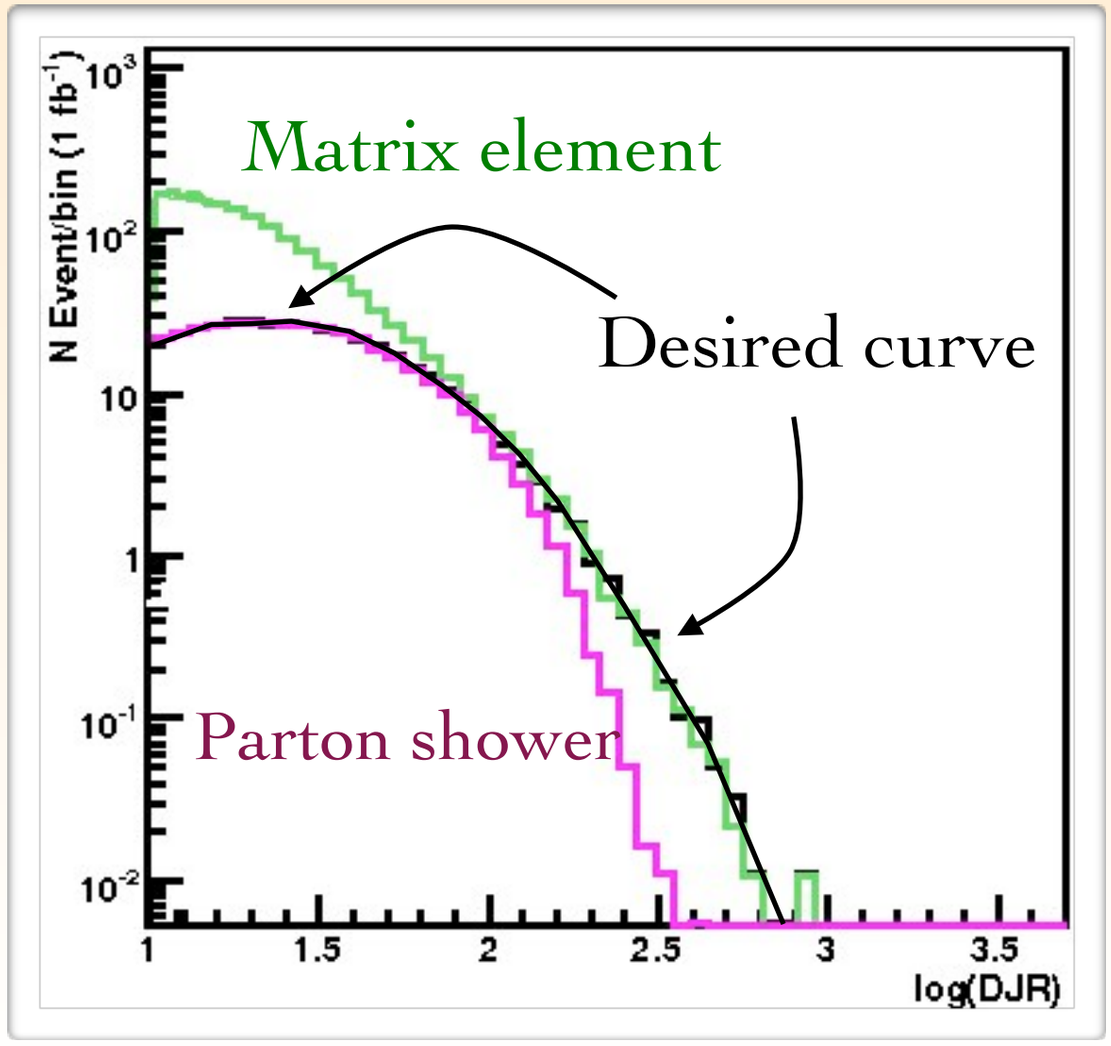

2nd QCD radiation jet in top pair production at the LHC

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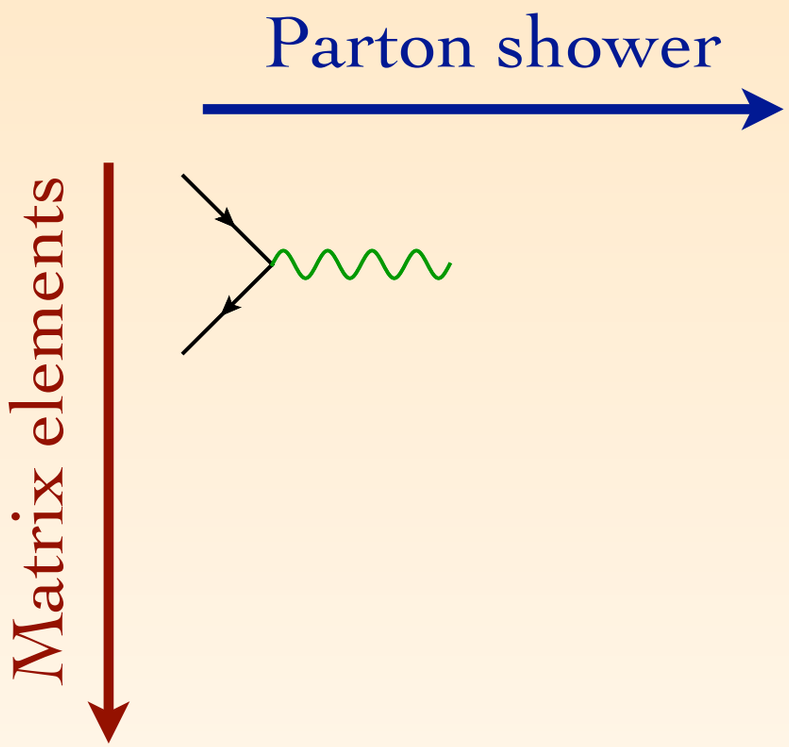

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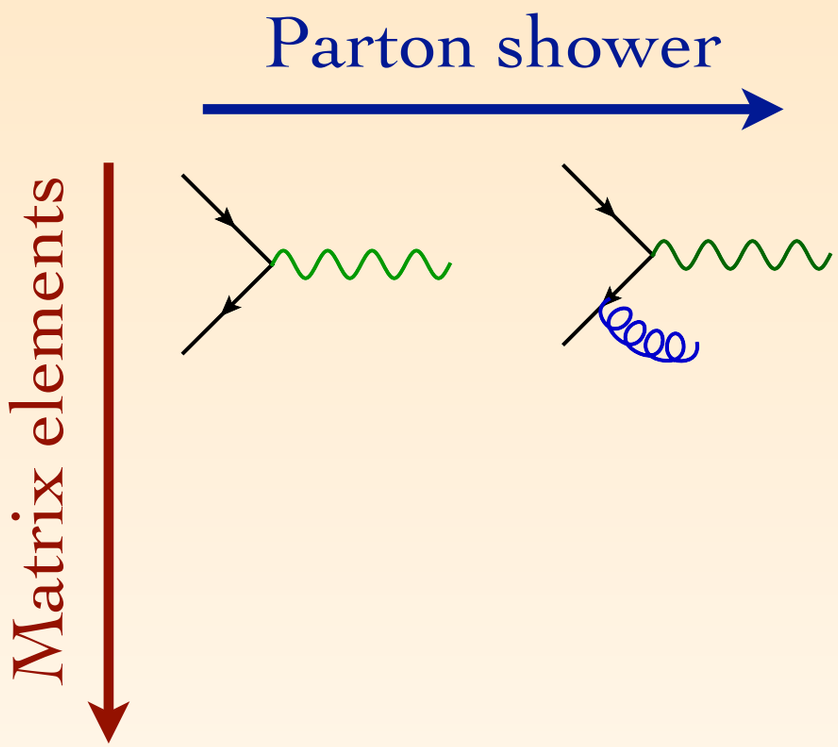

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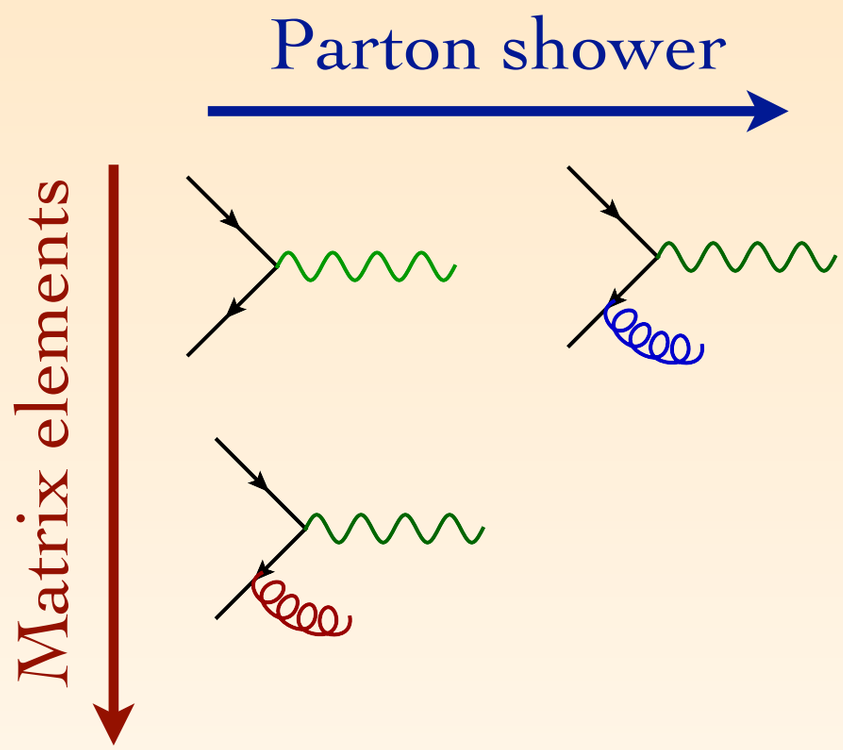

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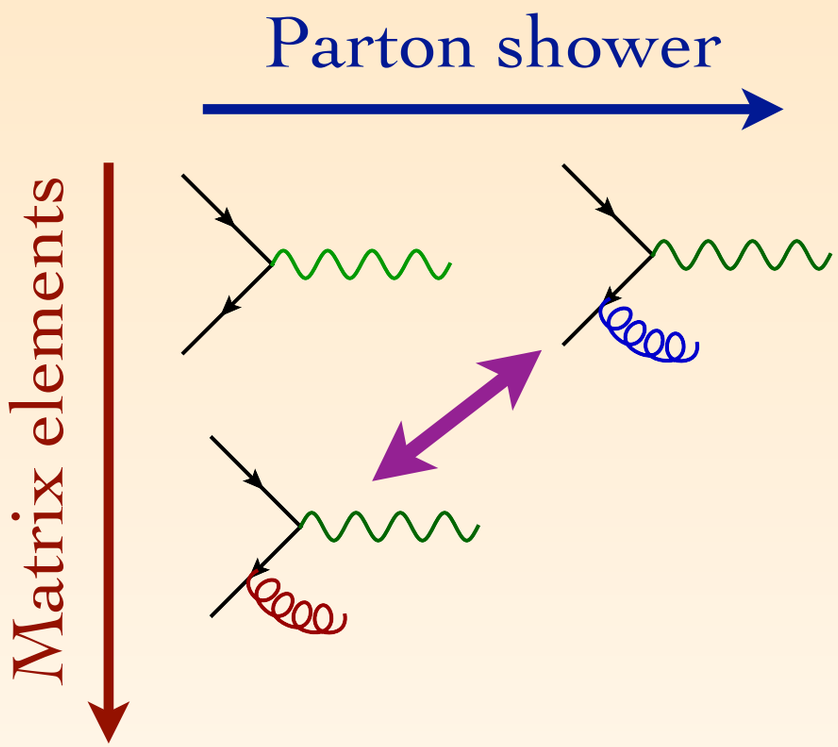

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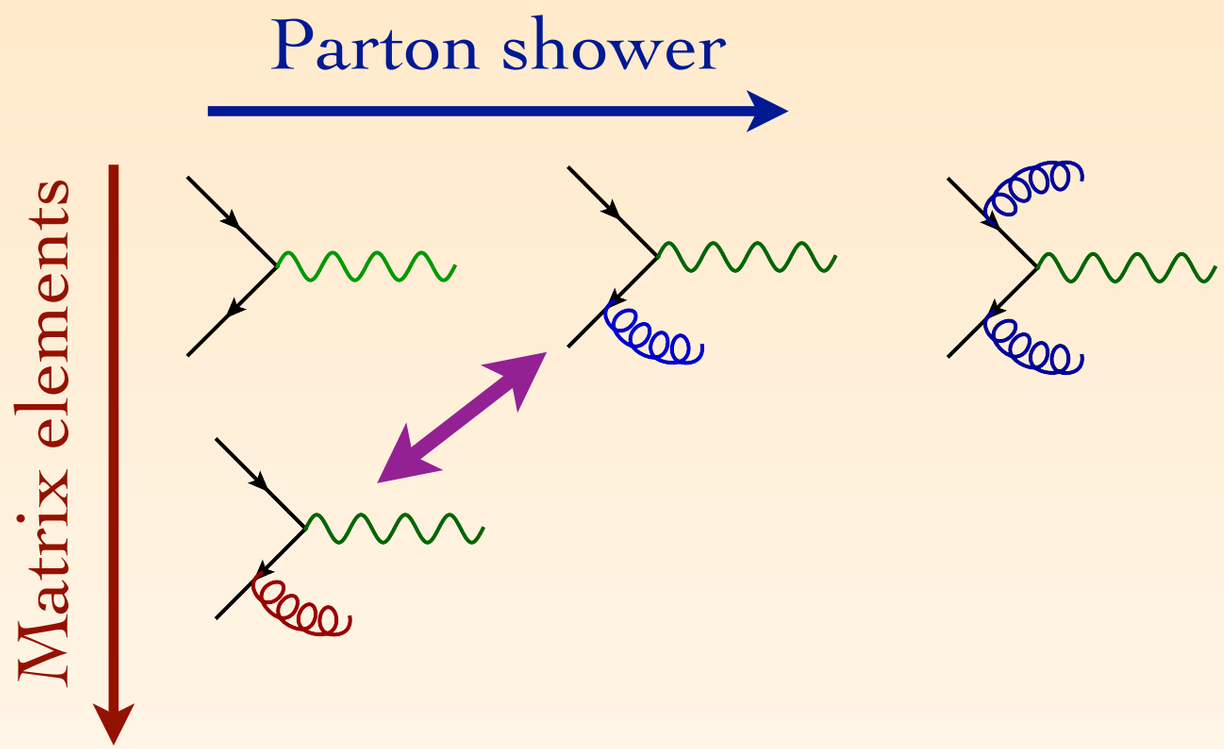

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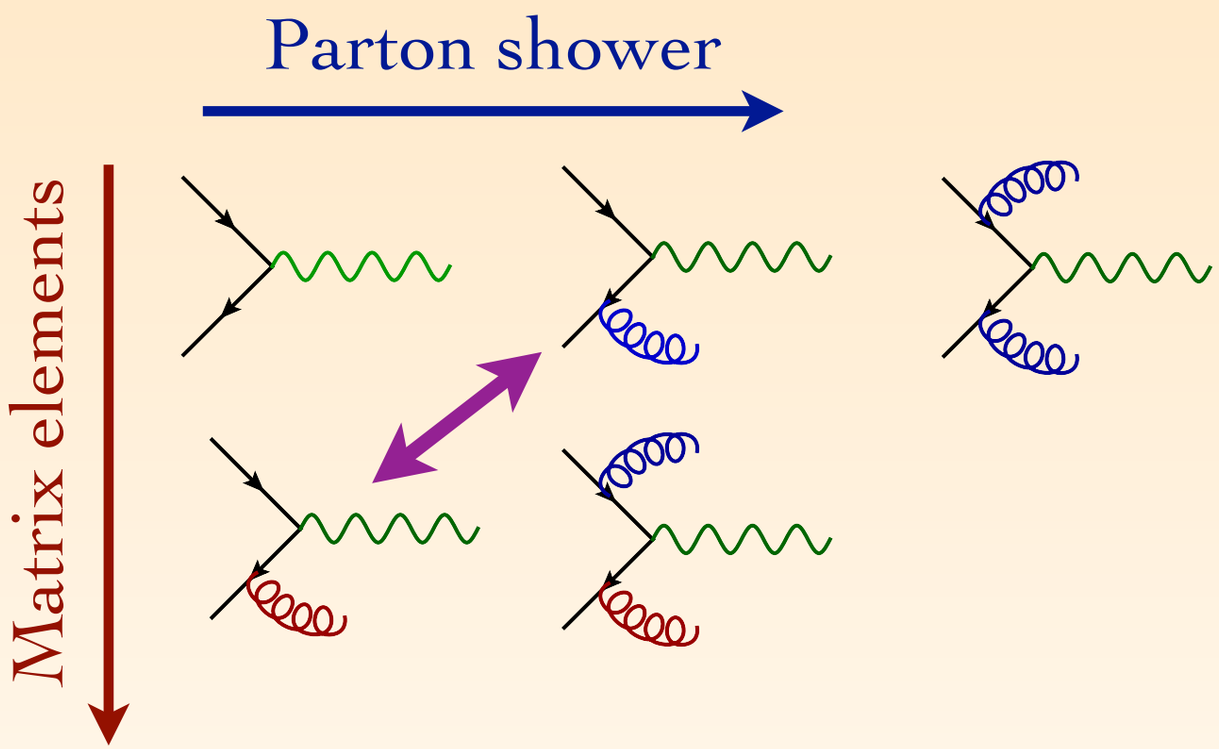

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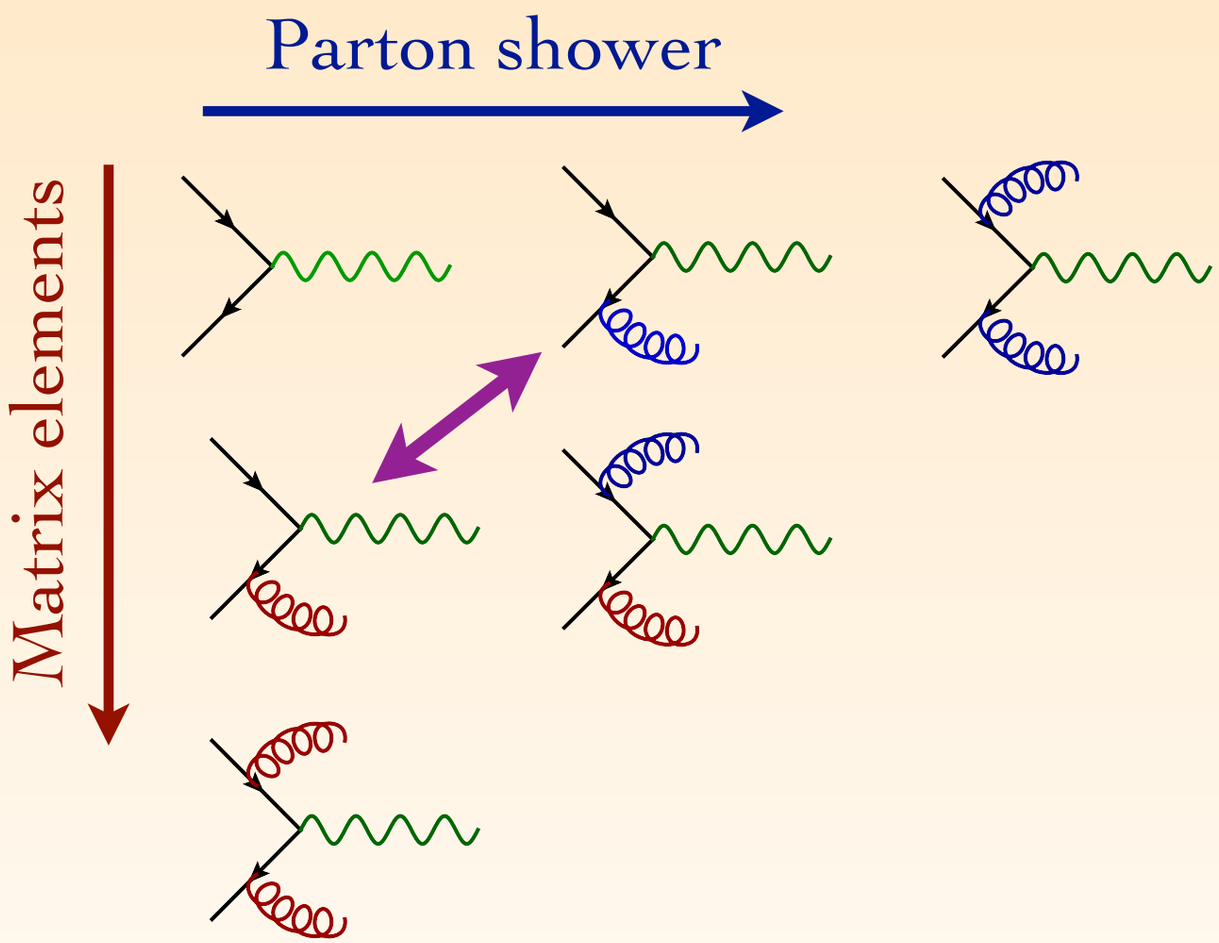

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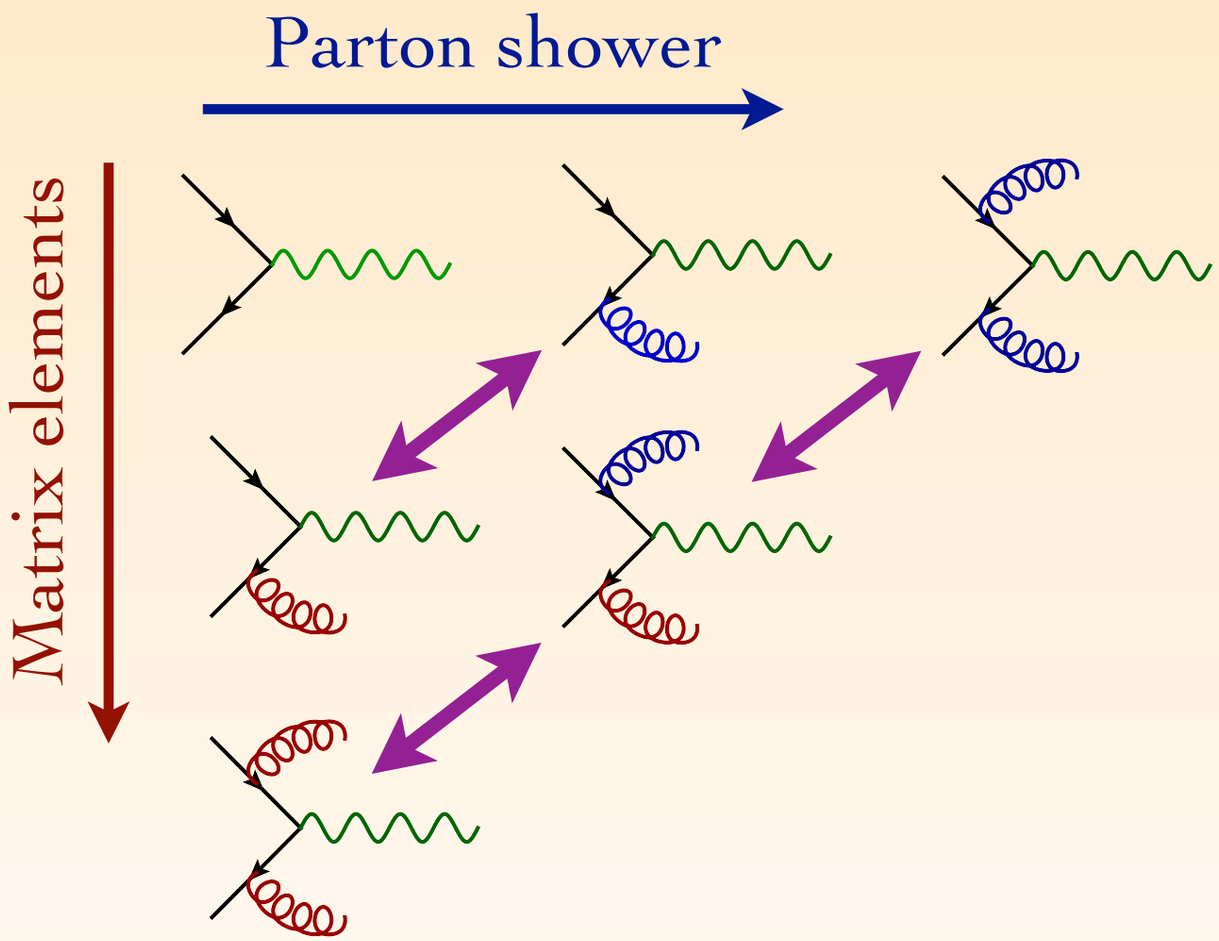

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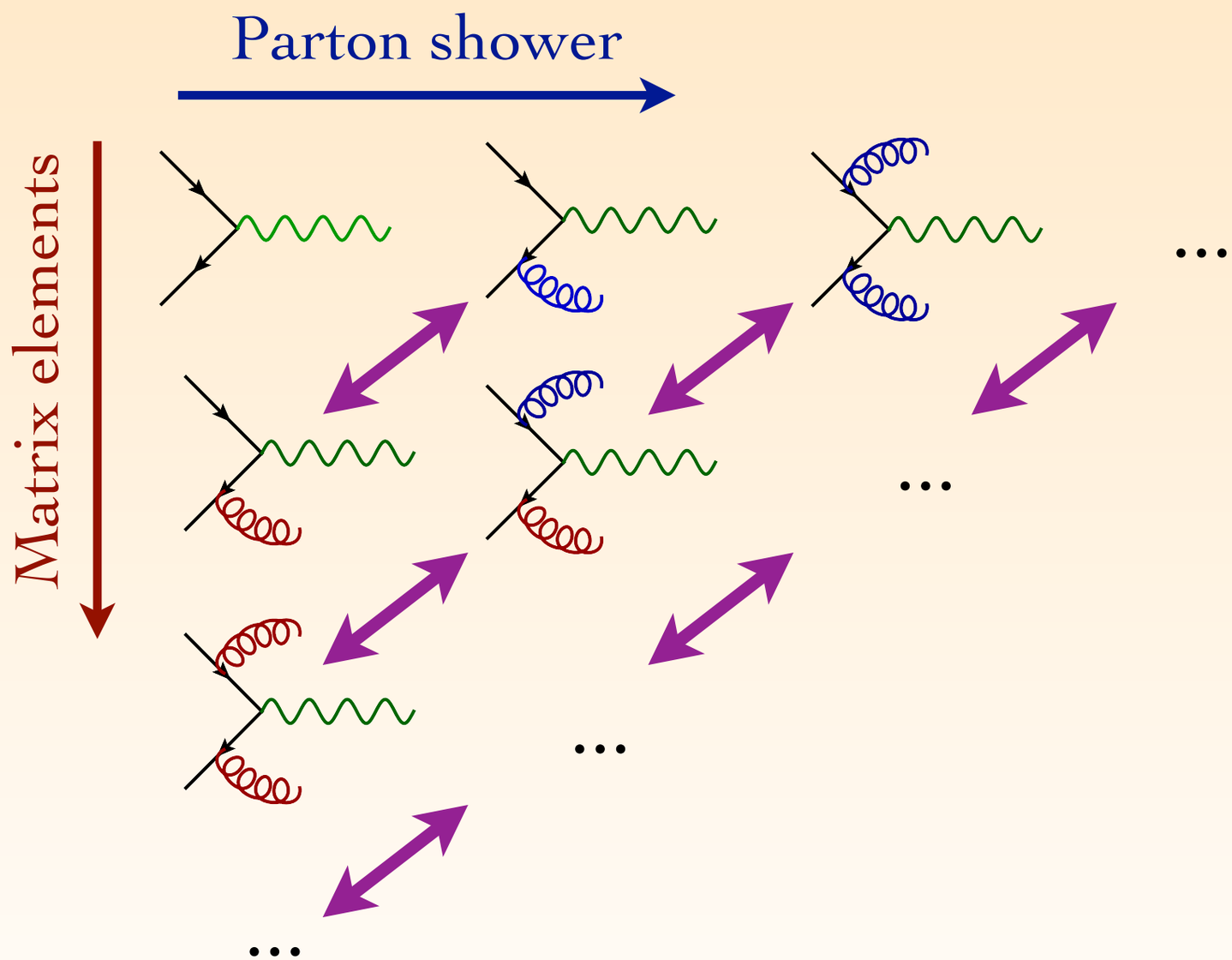

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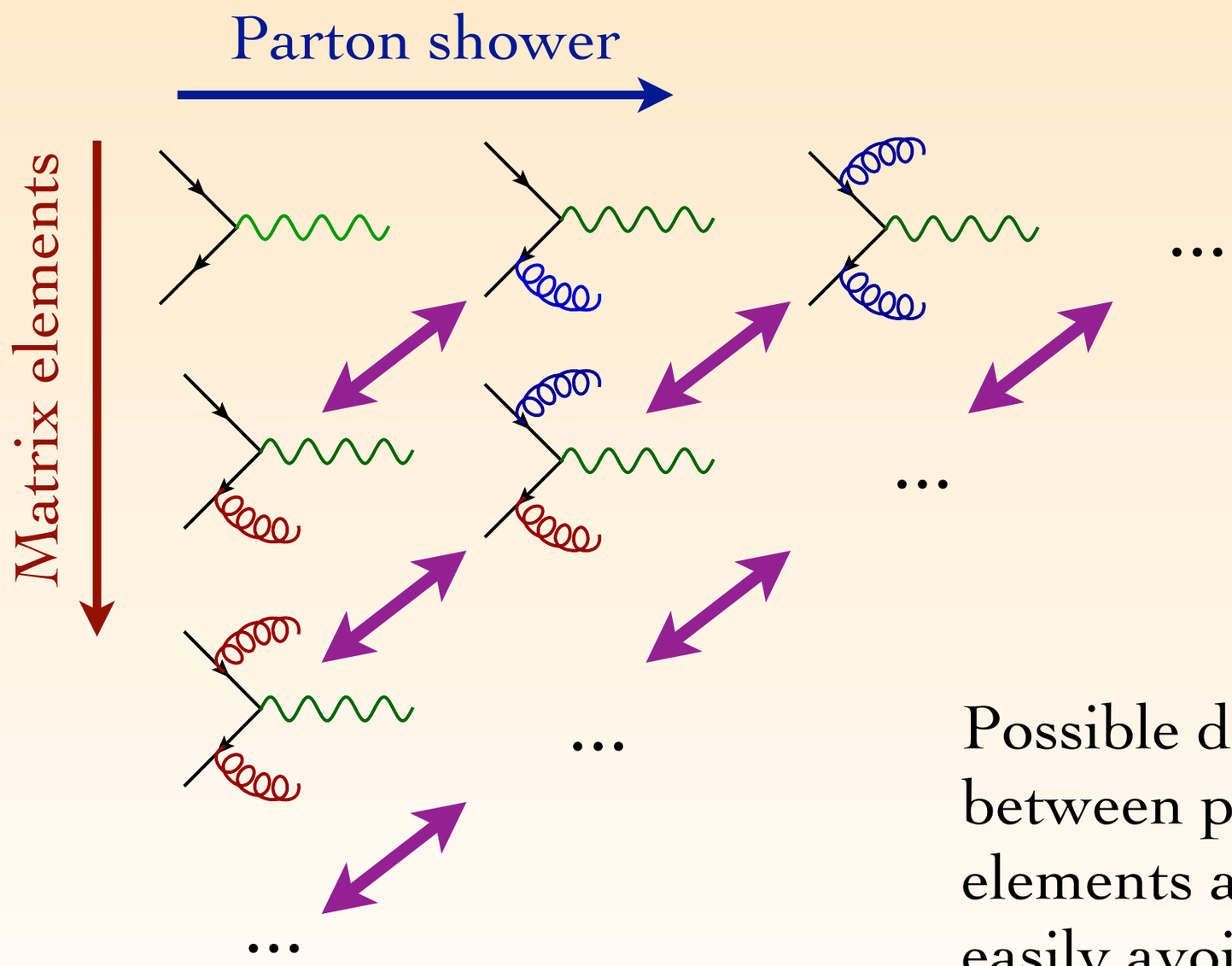

Possible double counting between partons from matrix elements and parton shower easily avoided by applying a cut in phase space

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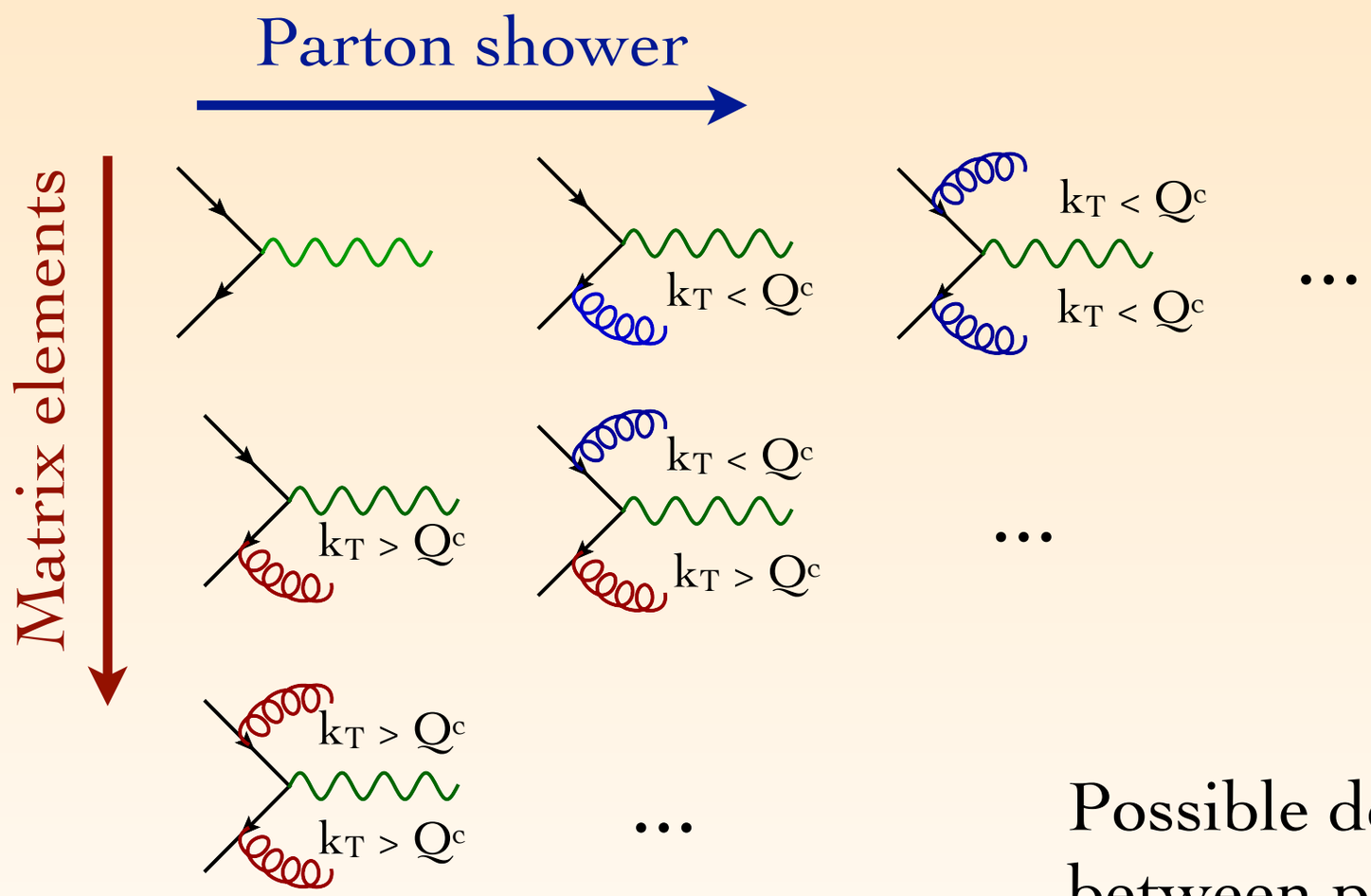
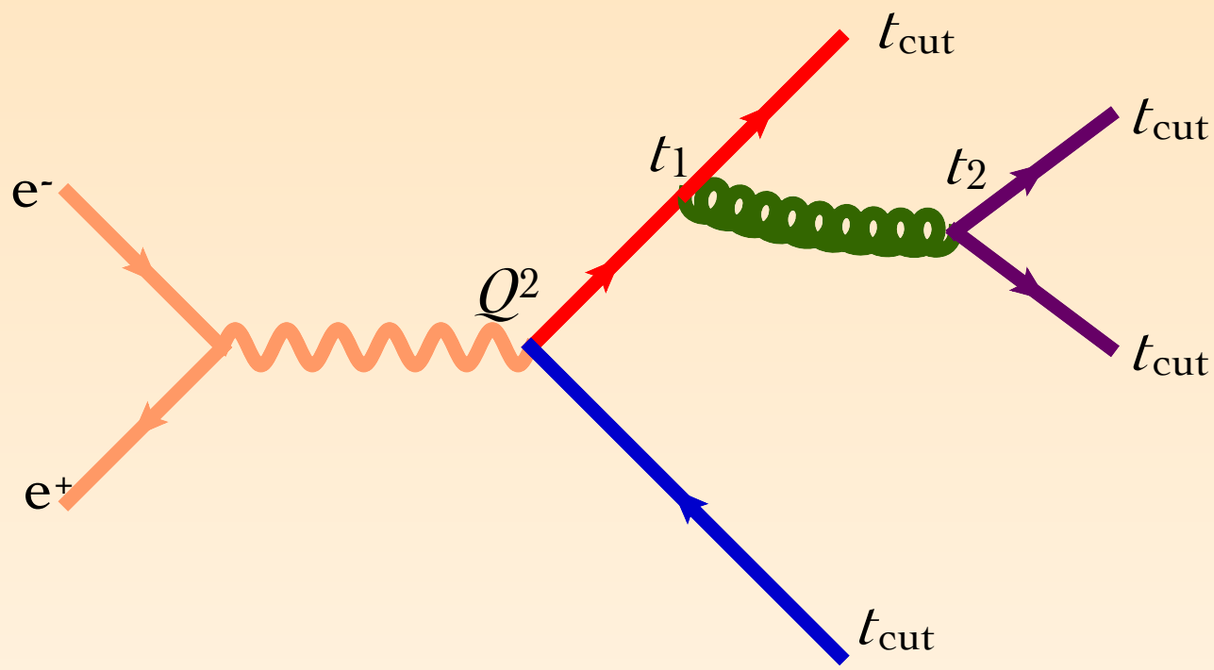


Possible double counting between partons from matrix elements and parton shower easily avoided by applying a cut in phase space

Merging ME with PS

- So double counting no problem, but what about getting smooth distributions that are independent of the precise value of Q^c?
- Below cutoff, distribution is given by PS
  - need to make ME look like PS near cutoff
- Let's take another look at the PS!

Merging ME with PS



- How does the PS generate the configuration above (i.e. starting from e^+e^- -> qqbar events)?
- Probability for the splitting at t_1 is given by

$$(\Delta_q(Q^2, t_1))^2 \frac{\alpha_s(t_1)}{2\pi} P_{gq}(z)$$

and for the whole tree

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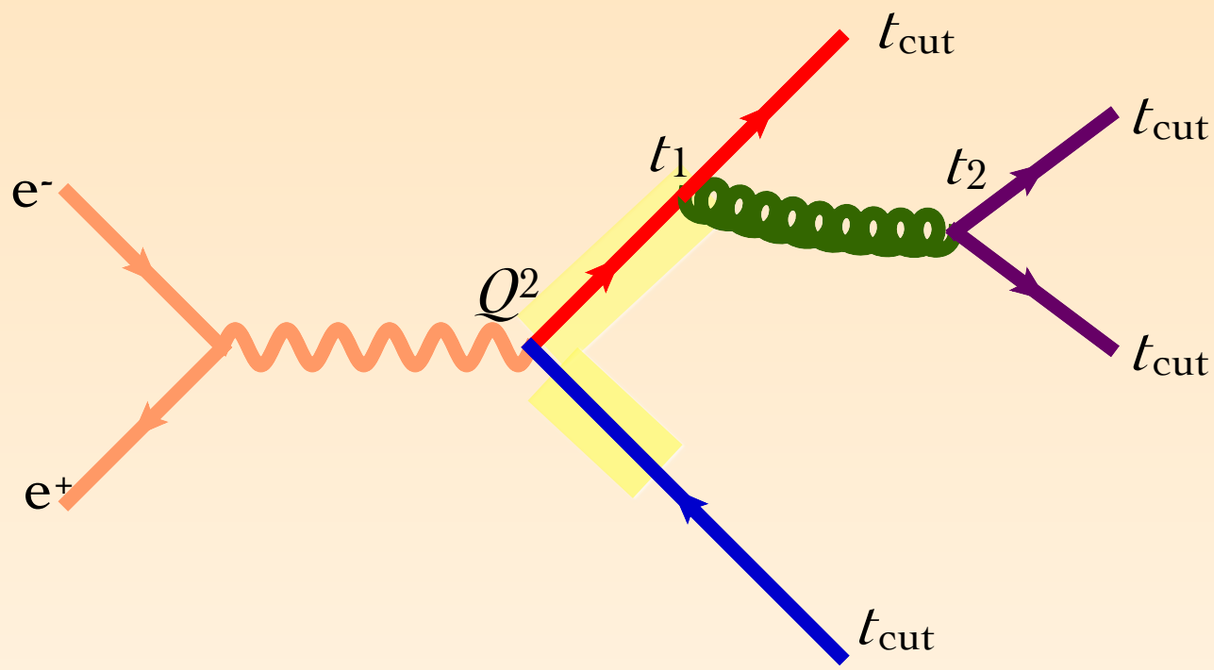

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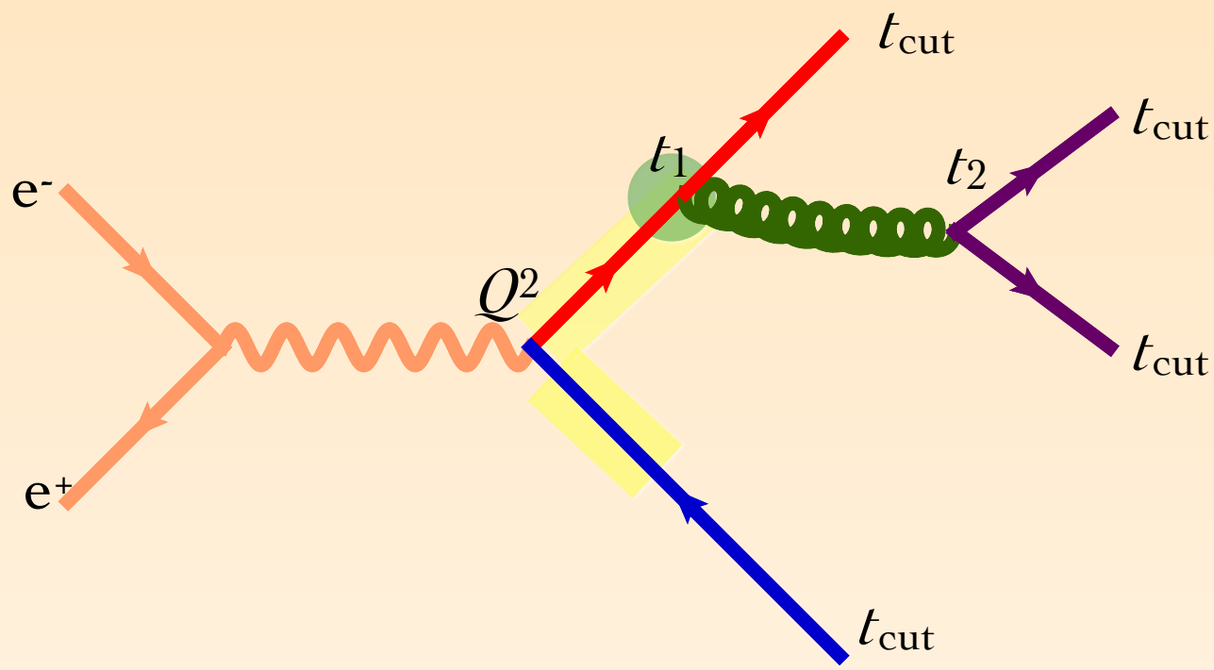

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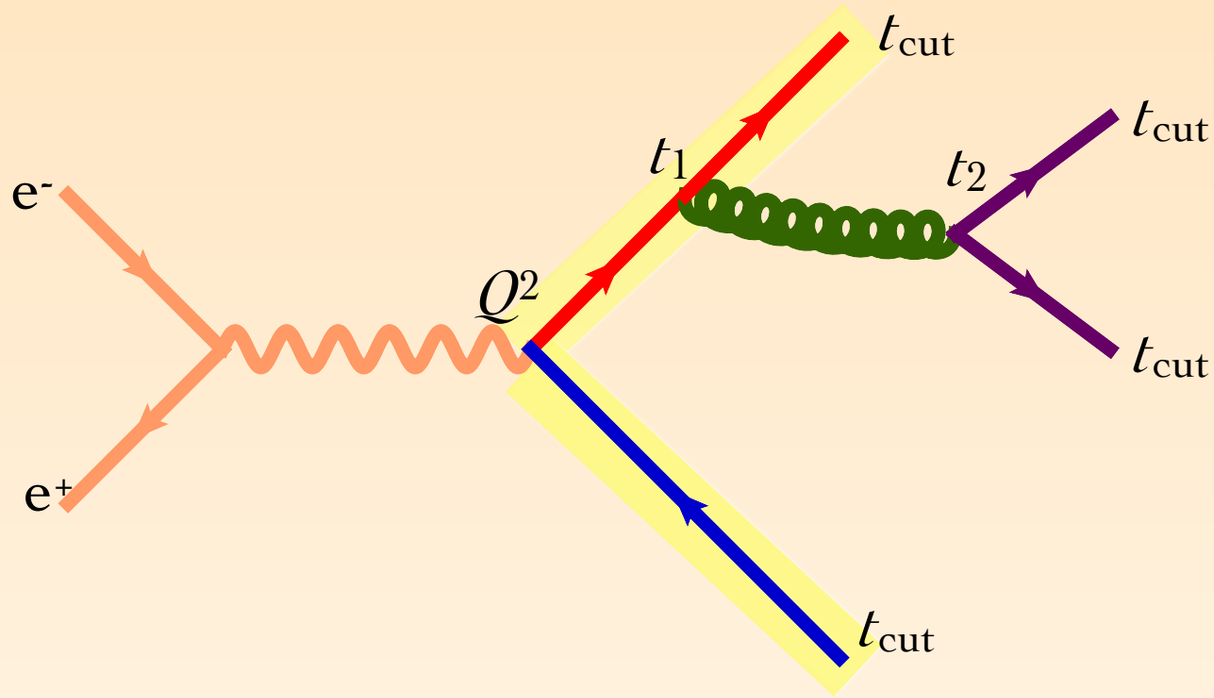

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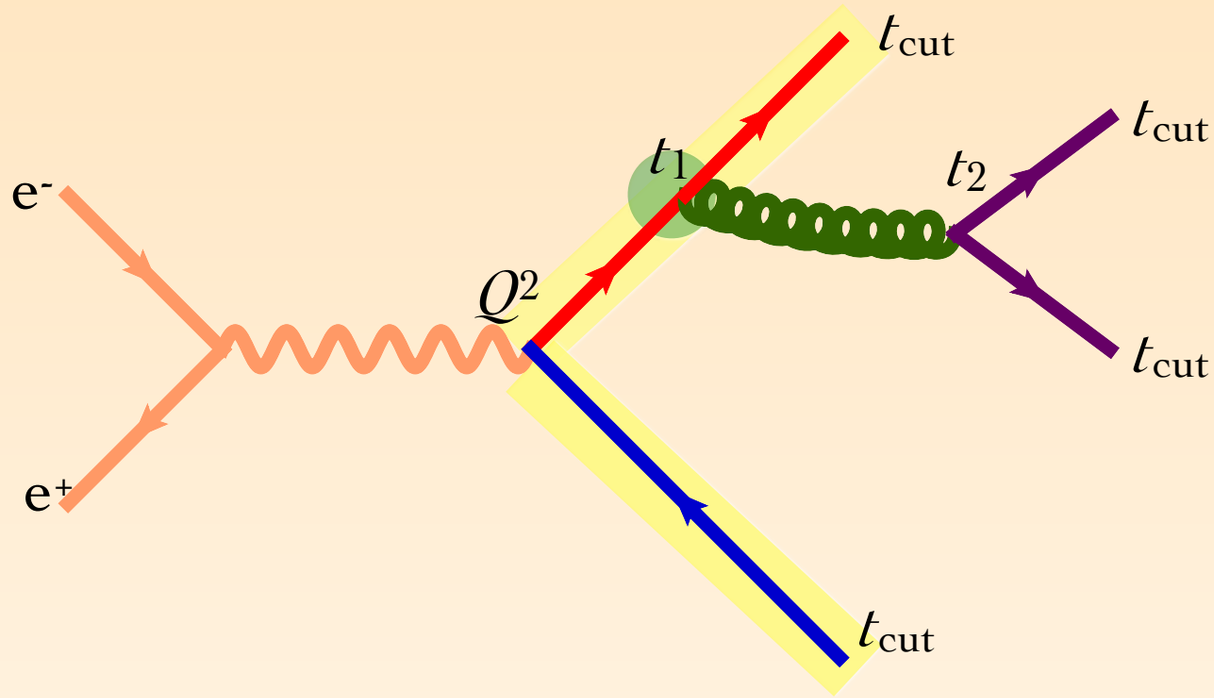

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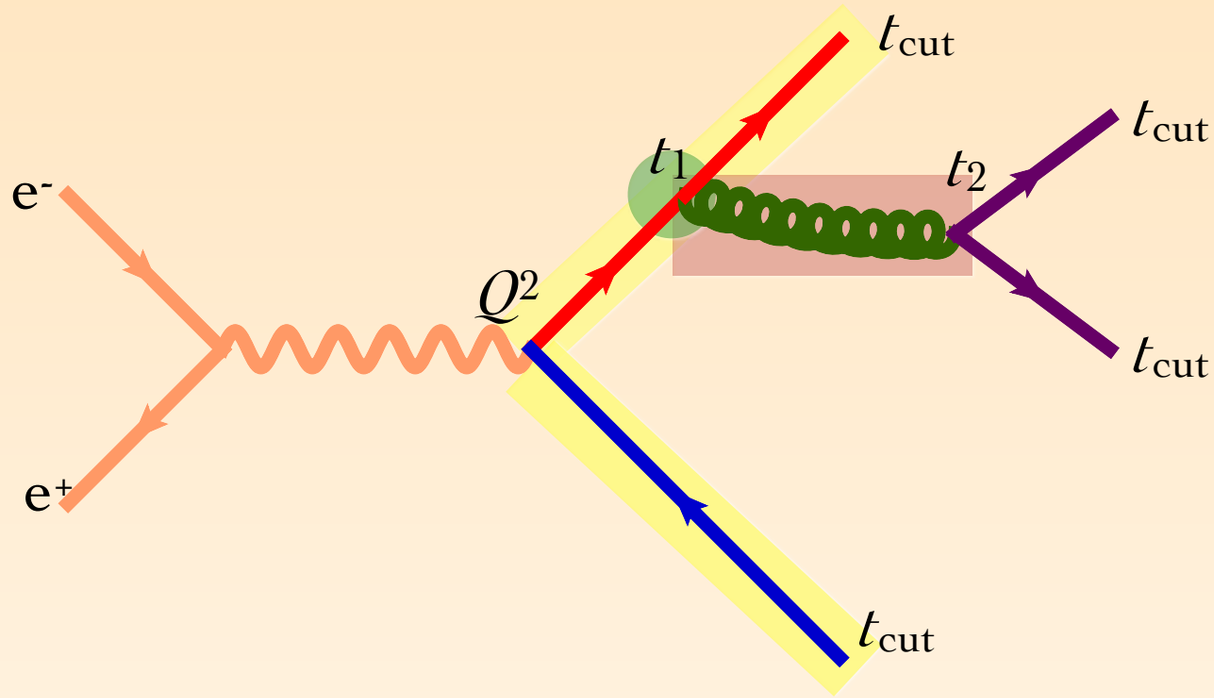

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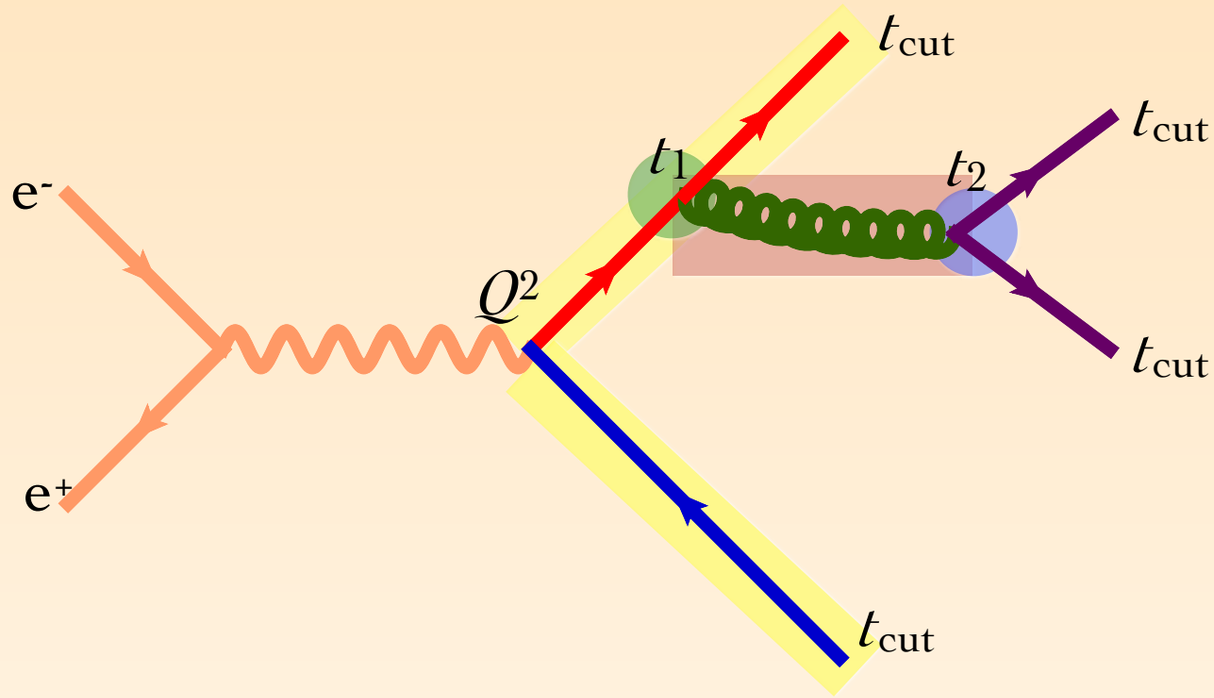

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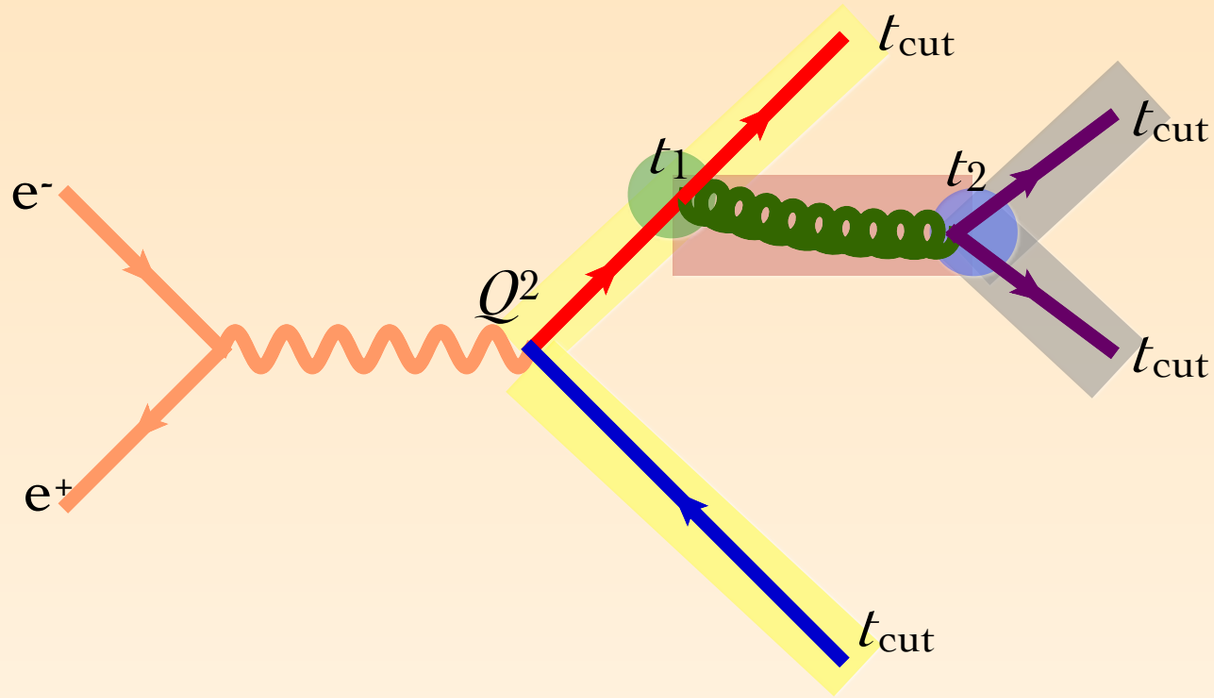

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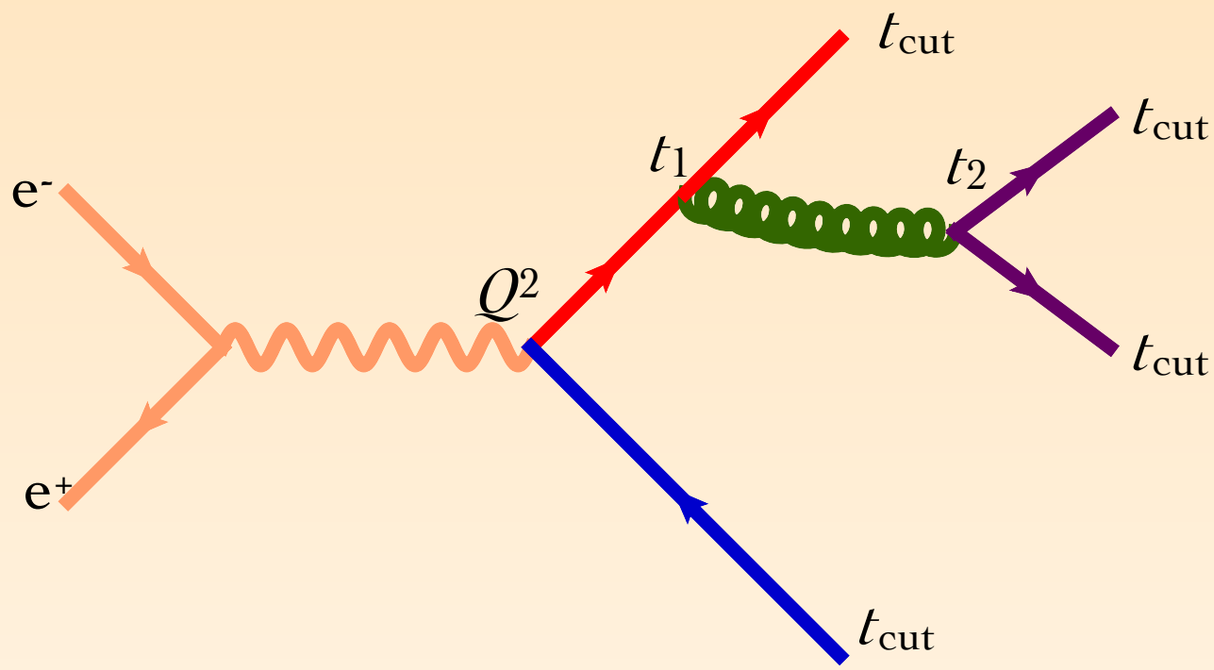

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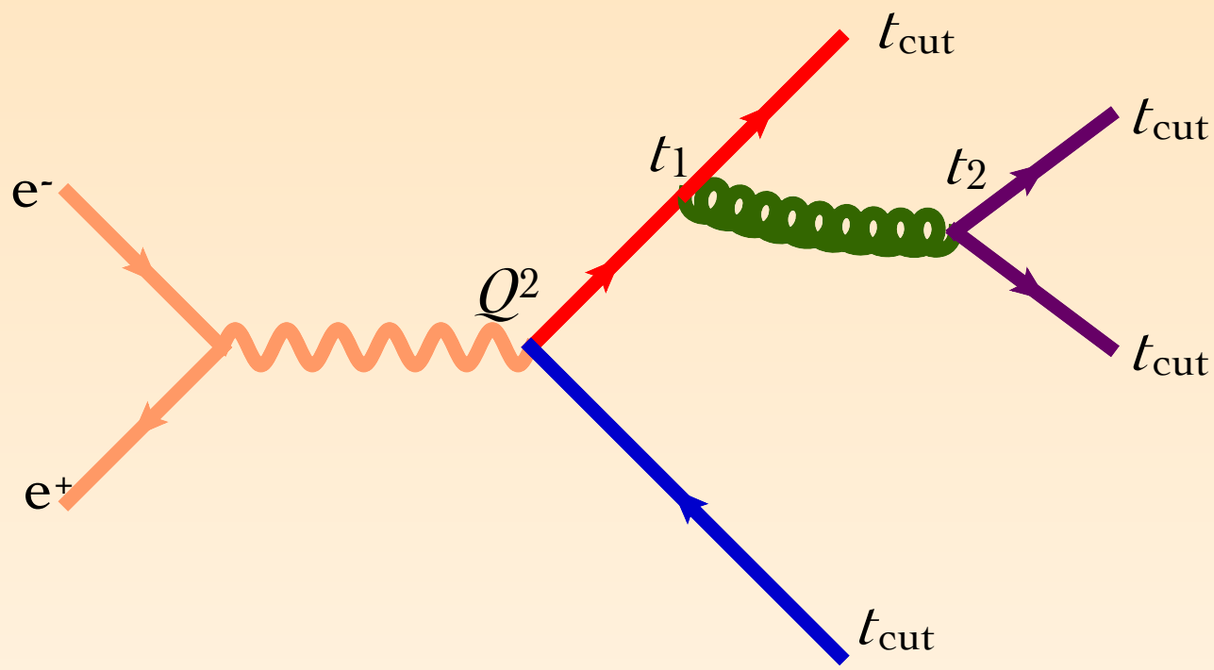

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Leading Logarithmic approximation of the matrix element
BUT with α_s evaluated at the scale of each splitting

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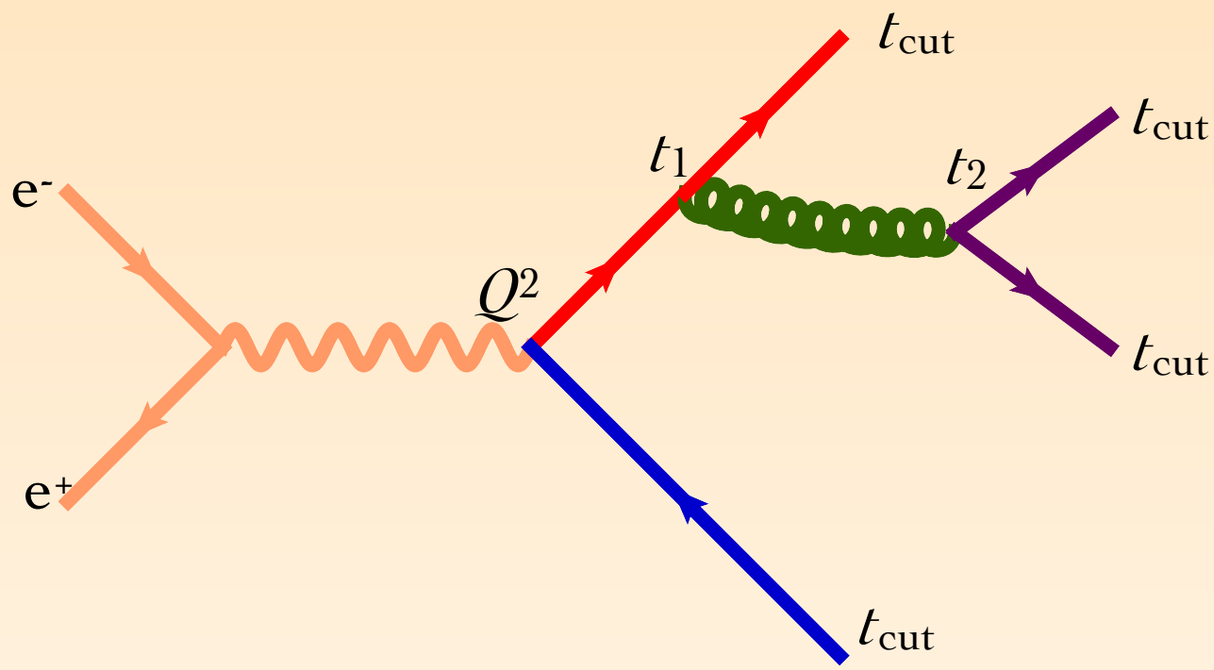

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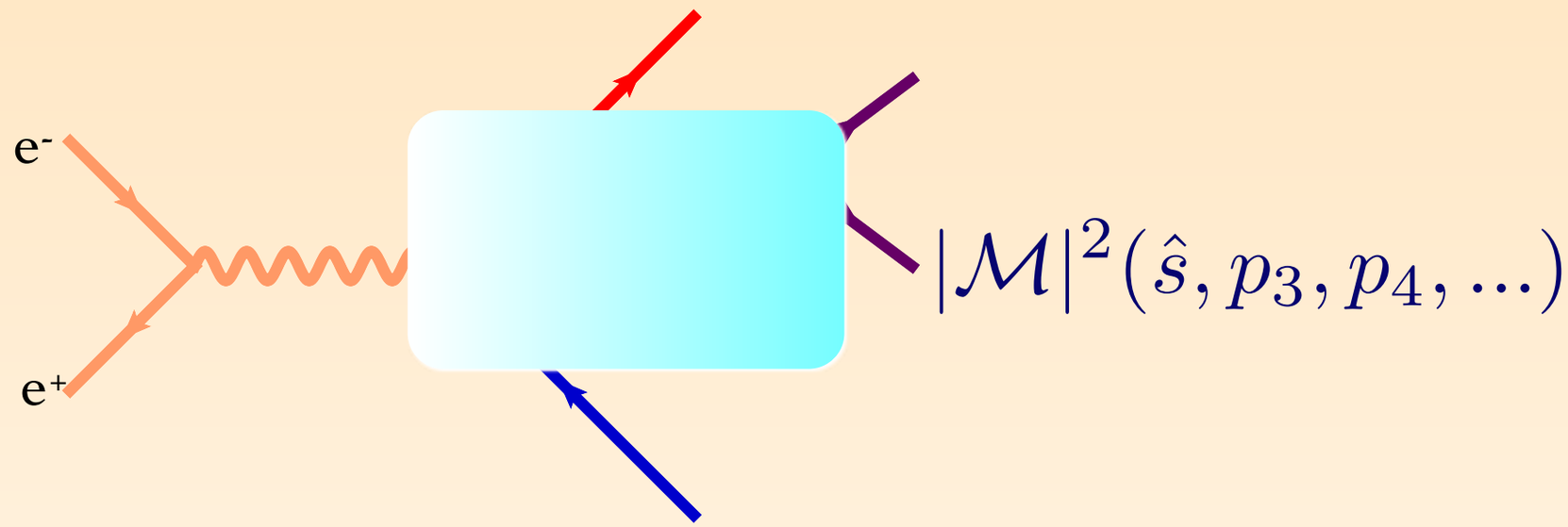
Sudakov suppression due to disallowing additional radiation
above the scale t_{cut}

Merging ME with PS



To get an equivalent treatment of the corresponding matrix element, do as follows:

1. Cluster the event using some clustering algorithm
   - this gives us a corresponding "parton shower history"
2. Reweight α_s in each clustering vertex with the clustering scale
   $$|\mathcal{M}|^2 \to |\mathcal{M}|^2 \frac{\alpha_s(t_1)}{\alpha_s(Q^2)} \frac{\alpha_s(t_2)}{\alpha_s(Q^2)}$$
3. Use some algorithm to apply the equivalent Sudakov suppression $(\Delta_q(Q^2, t_{\text{cut}}))^2 \Delta_g(t_1, t_2)(\Delta_q(t_2, t_{\text{cut}}))^2$

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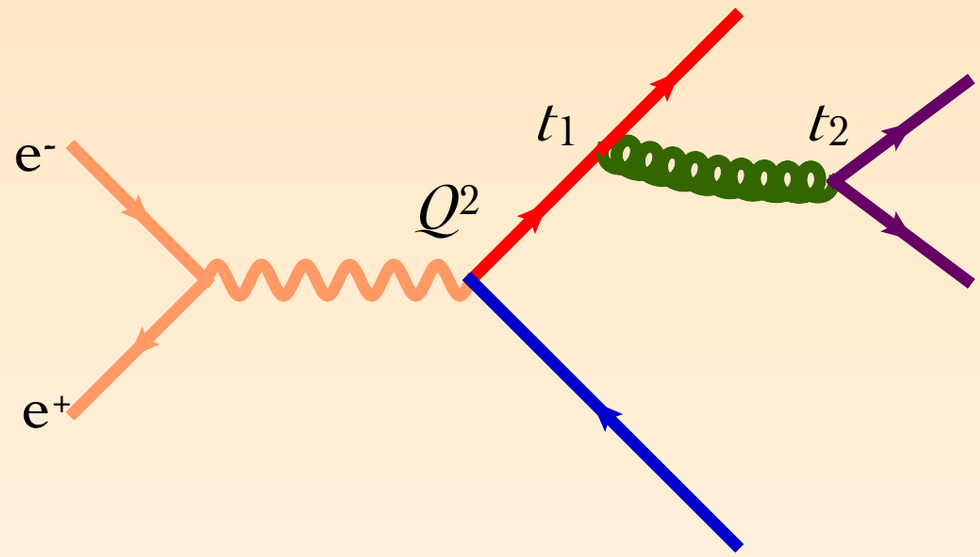

$$|\mathcal{M}|^2(\hat{s}, p_3, p_4, \ldots)$$

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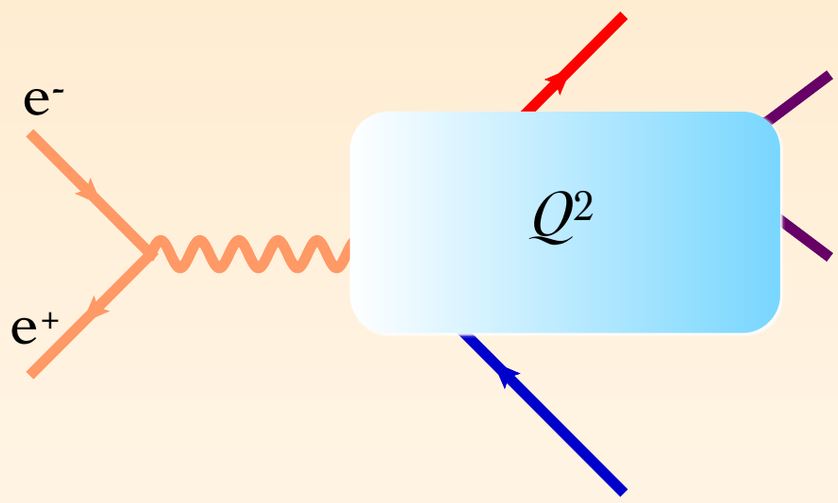
MLM matching

[M.L. Mangano, 2002, 2006]
[J. Alwall et al 2007, 2008]

- The simplest way to do the Sudakov suppression is to run the shower on the event, starting from t_0!



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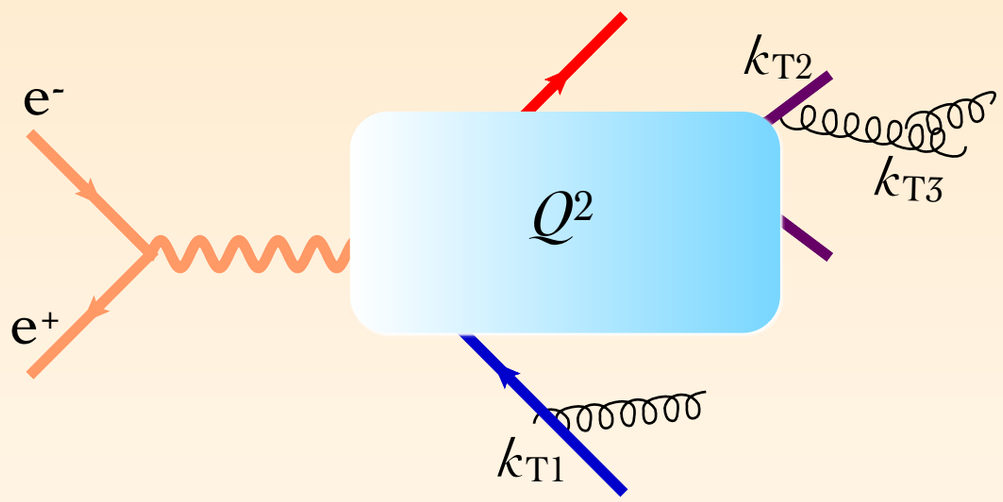

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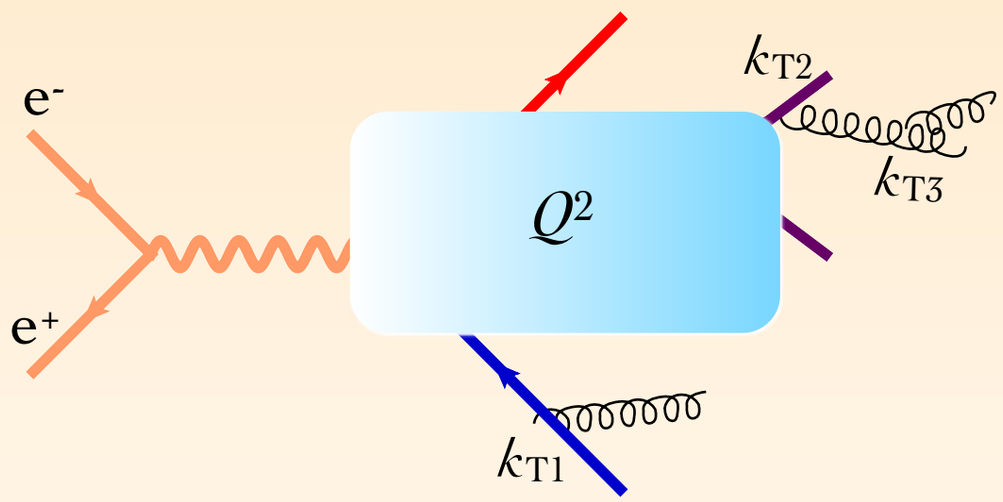
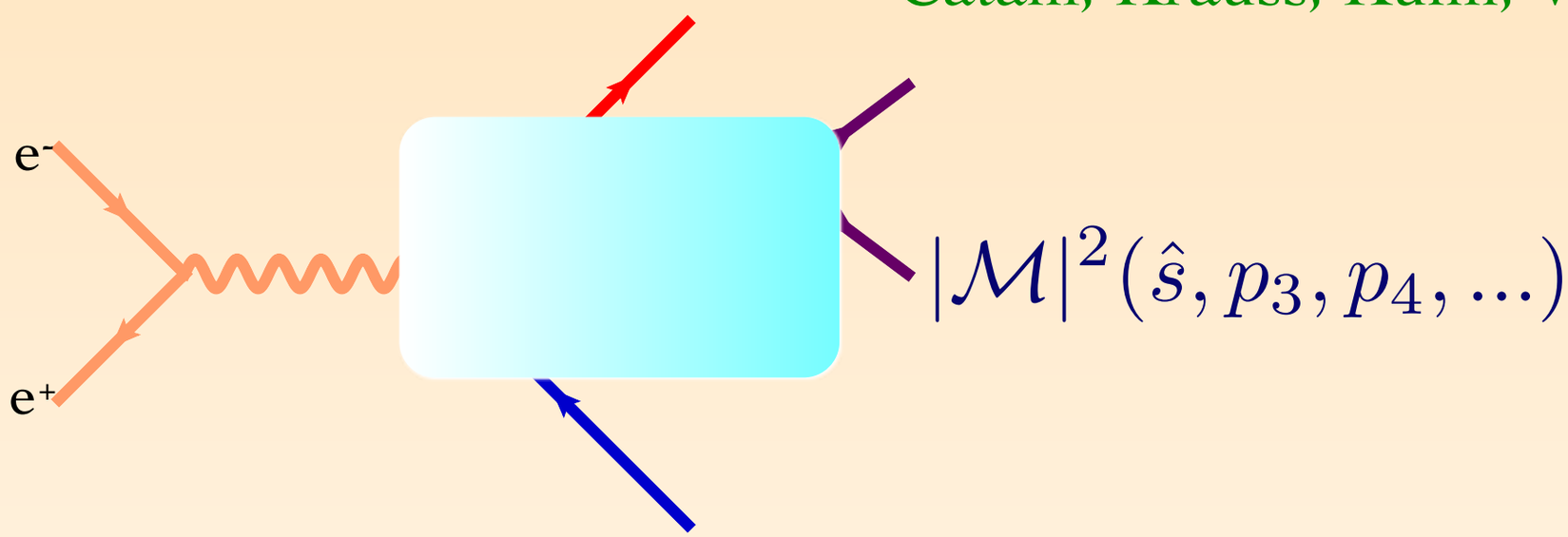


- If hardest shower emission scale $k_{T1} > t_{cut}$, throw the event away, if all $k_{T1,2,3} < t_{cut}$, keep the event
- The suppression for this is $(\Delta_q(Q^2, t_{cut}))^4$ so the internal structure of the shower history is ignored. In practice, this approximation is still pretty good
- Allows matching with any shower, without modifications!

CKKW MATCHING

Catani, Krauss, Kuhn, Webber [2001]



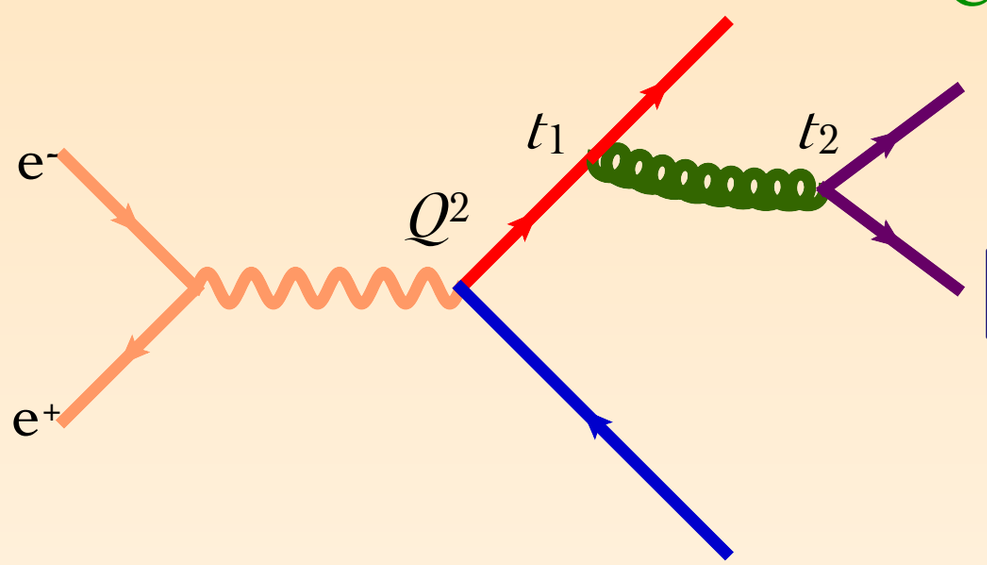
- Once the 'most-likely parton shower history' has been found, one can also reweight the matrix element with the Sudakov factors that give that history

$$(\Delta_q(Q^2, t_{\rm cut}))^2 \Delta_g(t_1, t_2)(\Delta_q(t_2, t_{\rm cut}))^2$$

- To do this correctly, must use same variable to cluster and define this sudakov as the one used as evolution parameter in the parton shower. Parton shower can start at $t_{\rm cut}$

CKKW MATCHING

Catani, Krauss, Kuhn, Webber [2001]



$$|\mathcal{M}|^2(\hat{s}, p_3, p_4, \ldots)$$

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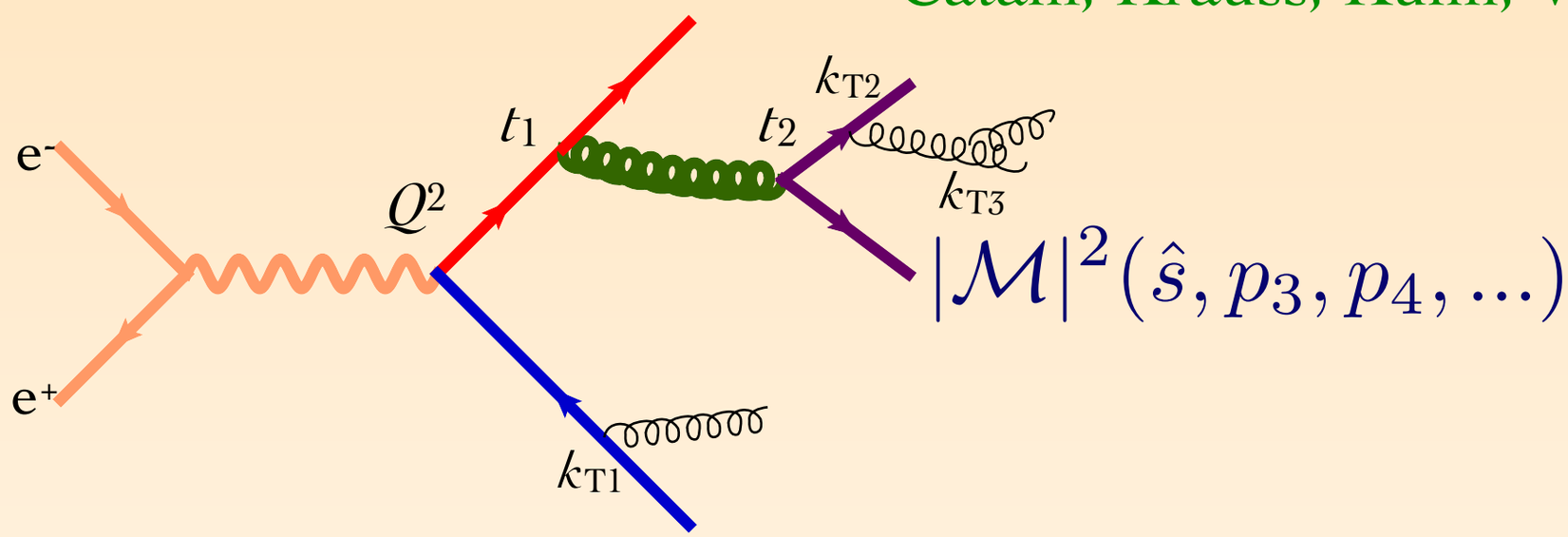

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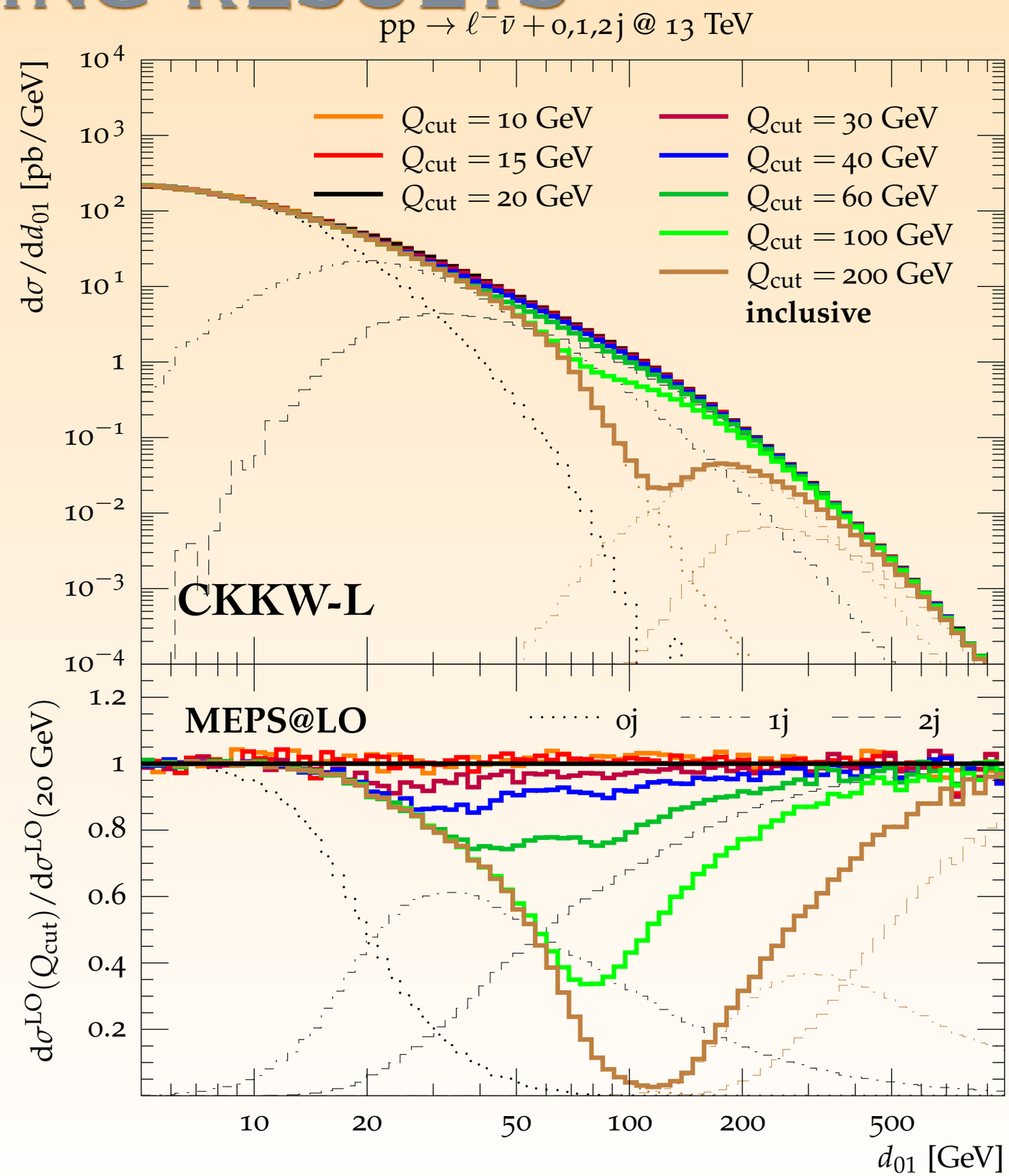
- To do this correctly, must use same variable to cluster and define this sudakov as the one used as evolution parameter in the parton shower. Parton shower can start at $t_{\rm cut}$

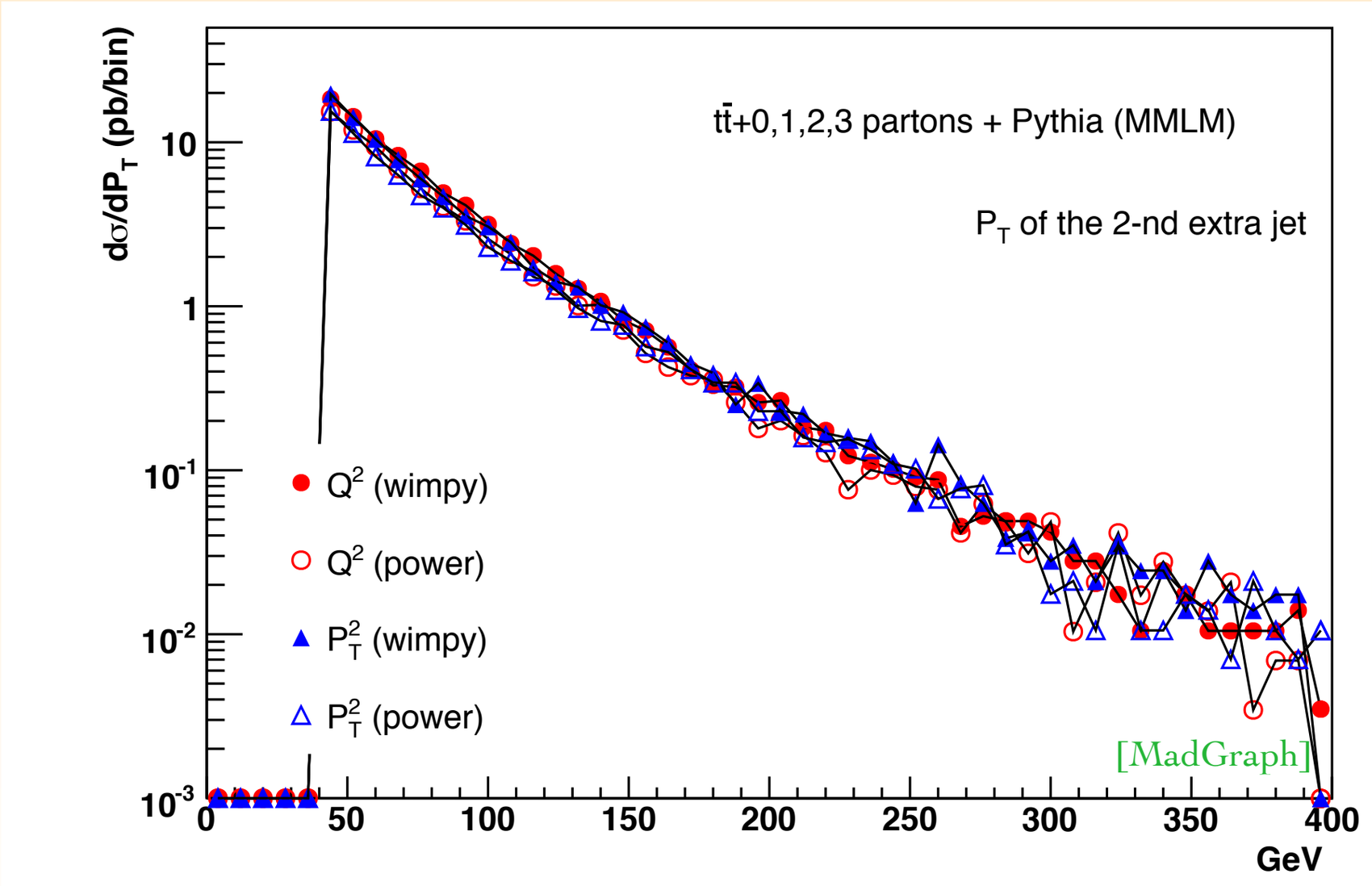
Matching results

- W+jets production: diff. jet rate for 0➞1 transition (~ p_T of hardest jet)
- Small dependence on the merging scale for small values, ~10%
  - When taken too large, the parton shower cannot fill the region all the way up to the merging scale anymore, leading to large deficits



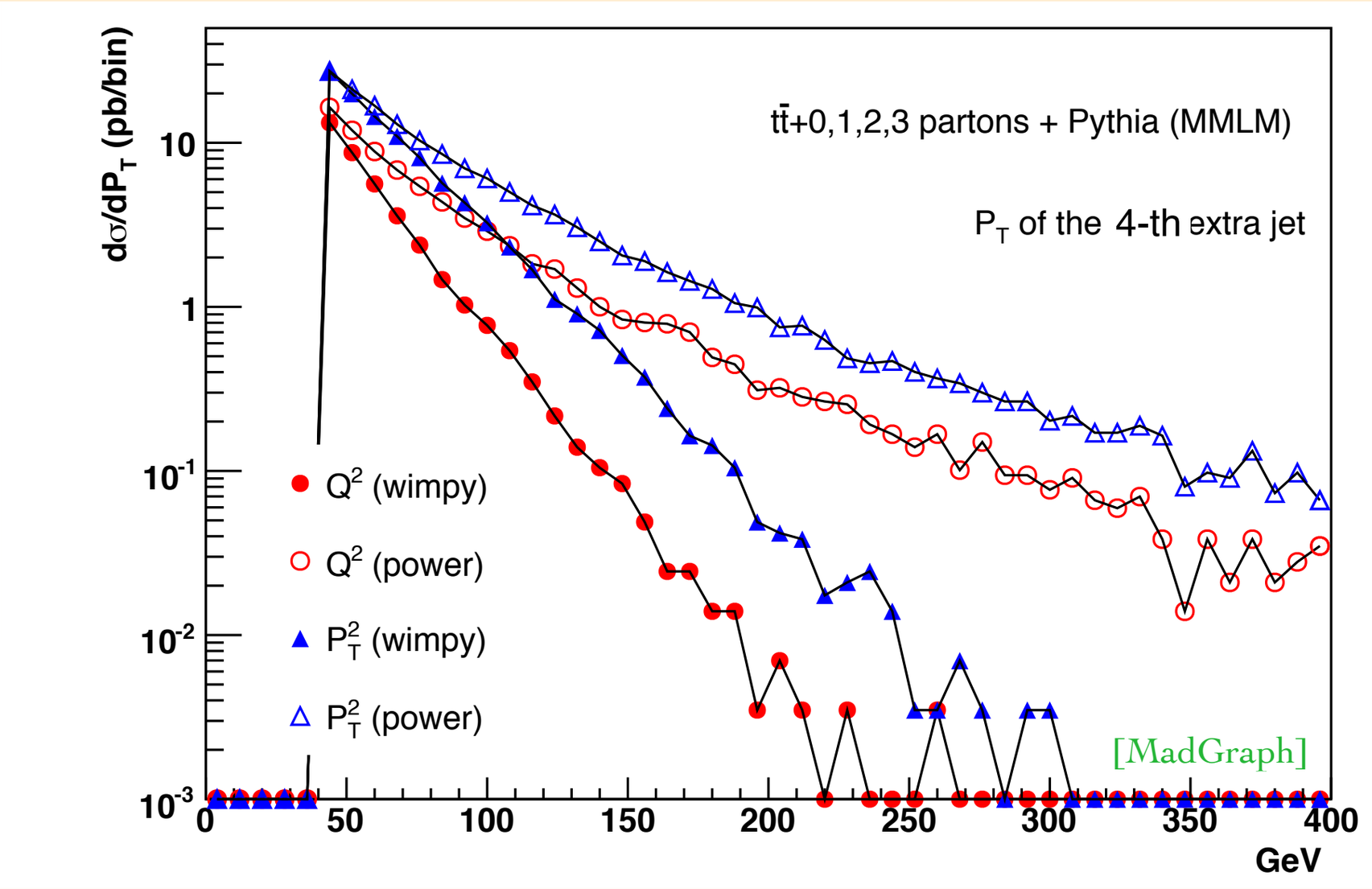
Beware: you only get what you generate...

For the 1-3rd extra jets: improved theory predictions reduce tuning dependence in generator, and therefore improve the accuracy of the predictions.



Beware: you only get what you generate…

However, the 4th hardest extra jet is still generated by the shower alone resulting in…



Summary

- Merging LO matrix elements with parton showers gives a consistent description of all the perturbative part of event generation
- Effectively two methods are available (MLM and CKKW) but both work on the same principles:
  - Introduce a merging scale "t_{cut}"
  - Use matrix elements where all partons are harder than "t_{cut}". Add Sudakov dampening to the matrix elements
  - Let the shower fill the region below the scale "t_{cut}"
- By using matrix elements, tuning dependence of hard radiation is reduced and predictive power is increased
  - Warning: only for observables where the matrix elements are relevant…

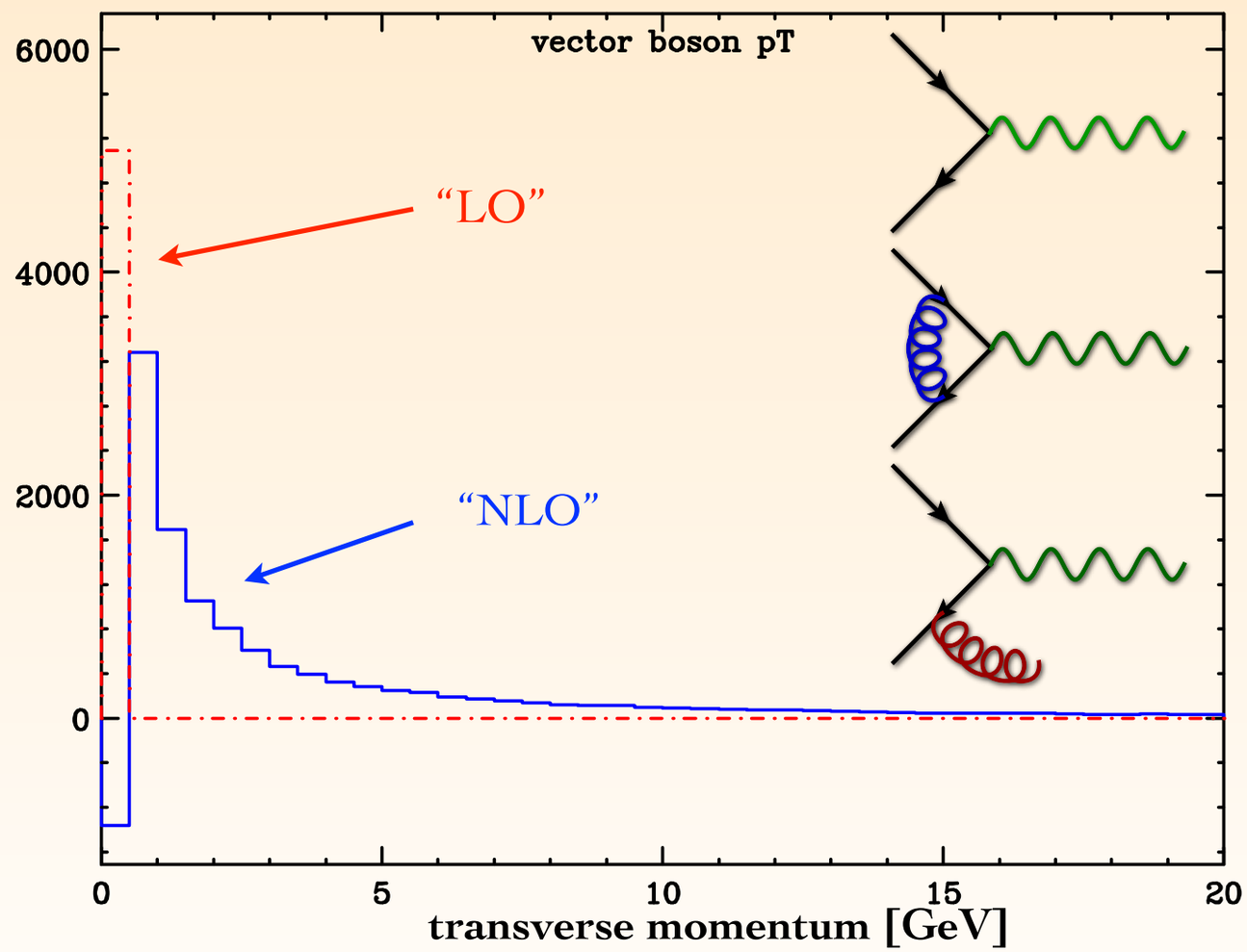
NLO+PS matching

Improving the formal accuracy of predictions

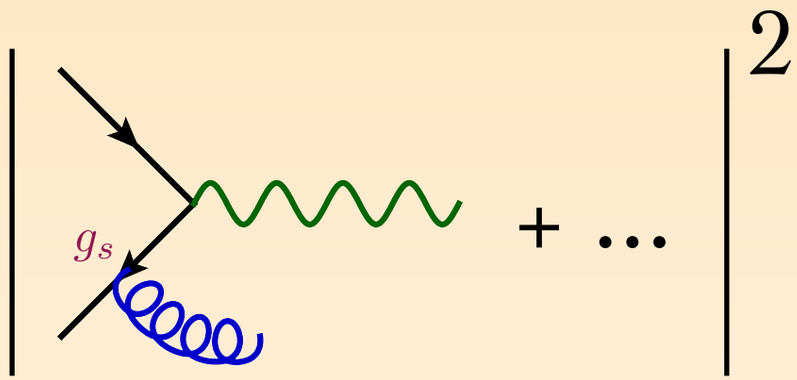
- Parton shower MC programs are only correct in the soft-collinear region. Hard radiation cannot be described correctly
- There are two ways to improve a Parton Shower Monte Carlo event generator with matrix elements:
  - NLO+PS matching: include full NLO corrections to the matrix elements to reduce 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
  - Combine the two above methods!

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

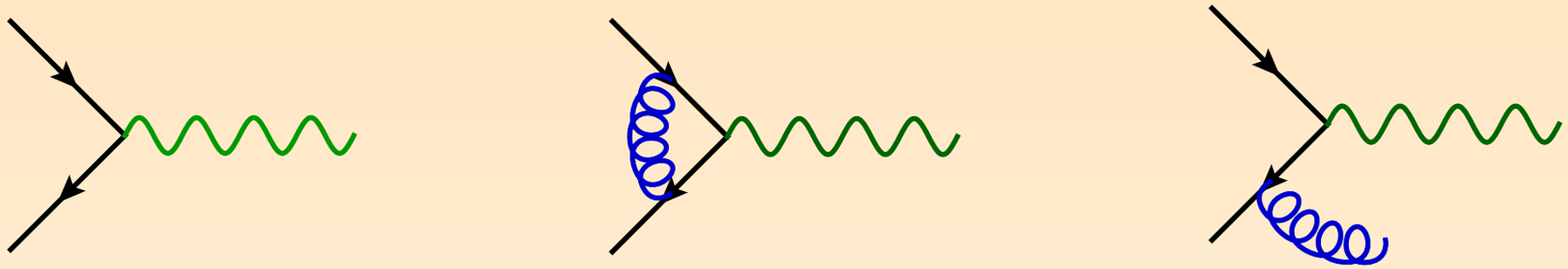


At NLO



- 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
- We can NOT use the same merging procedure as used at LO (MLM or CKKW): requiring that all partons should produce separate jets is not infrared safe
- 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

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

- We could try to shower them independently
- Let $I_{\mathrm{MC}}^{(k)}(O)$ 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

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

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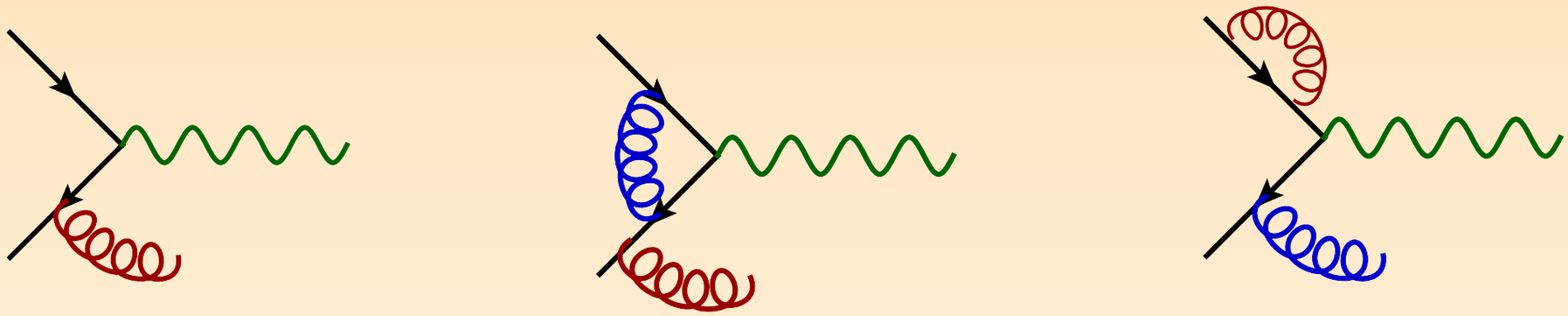

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Double counting

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

- But this is wrong!
- If you expand this equation out up to NLO, there are more terms then there should be and the total rate does not come out correctly
- Schematically $I_{\mathrm{MC}}^{(k)}(O)$ for 0 and 1 emission is given by

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

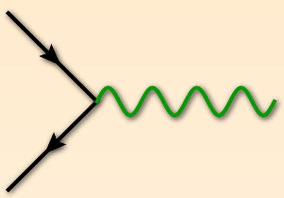
- And Δ is the Sudakov factor

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

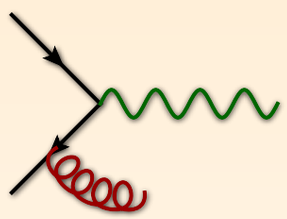
Sources of double counting

Parton shower

Born+Virtual:



Real emission:



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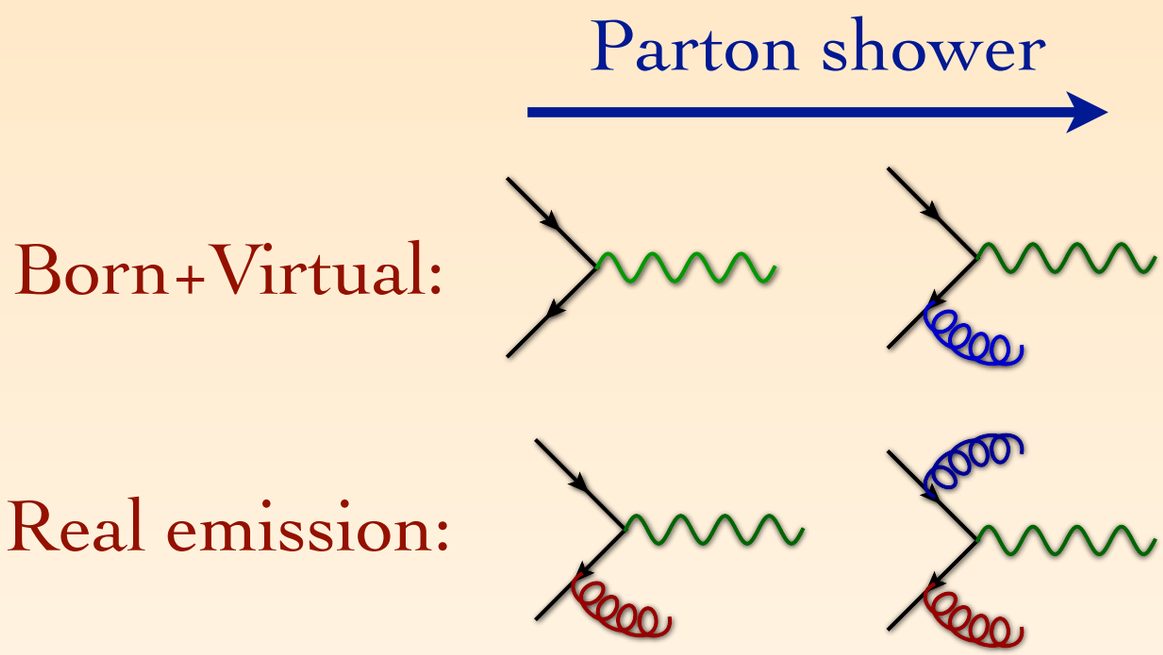

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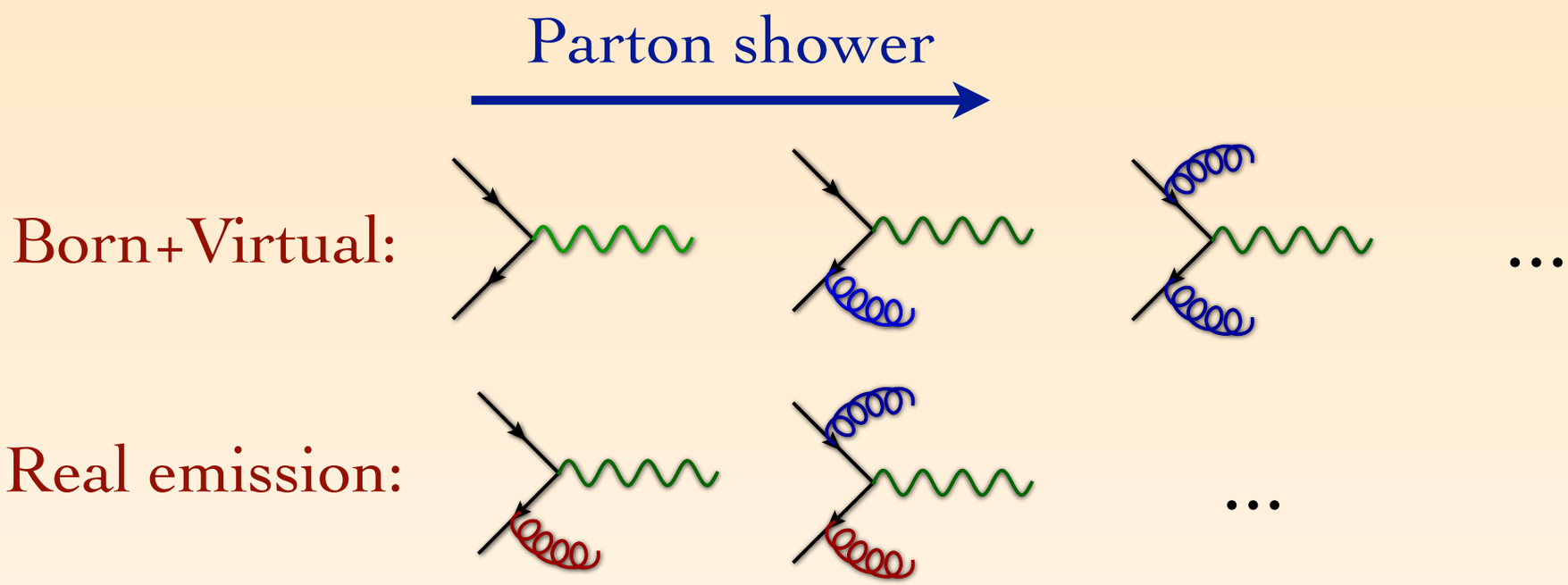

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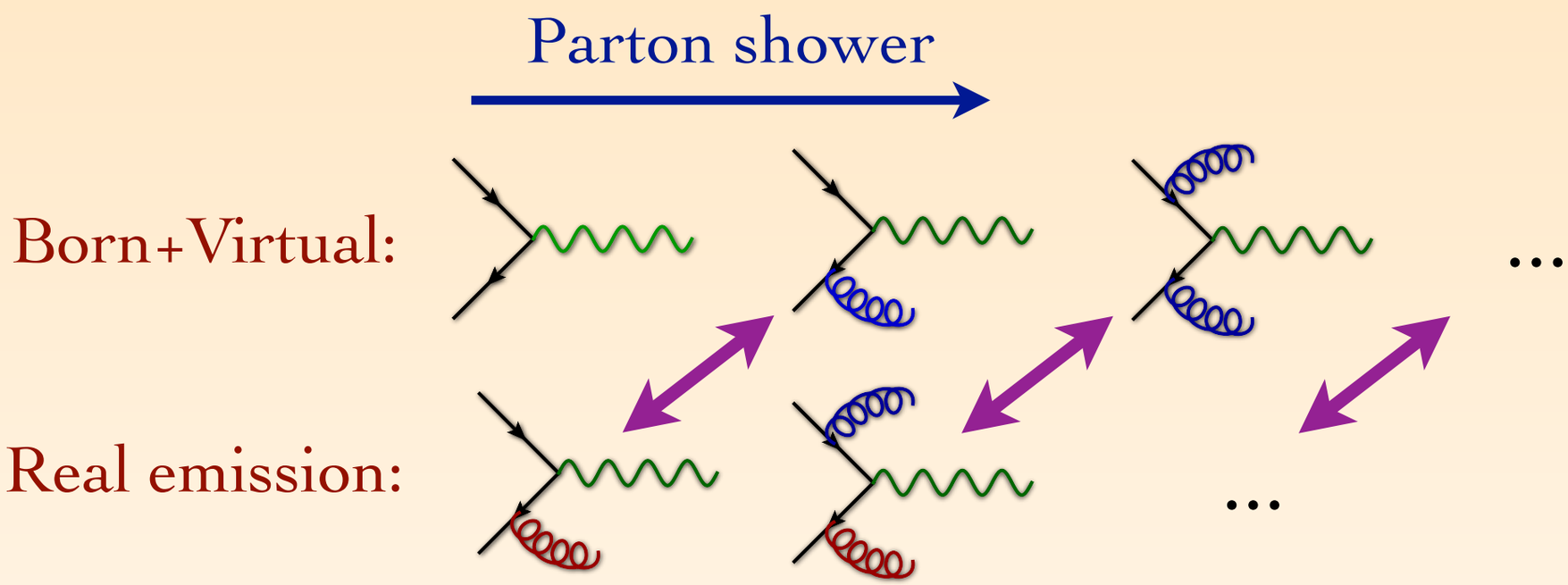
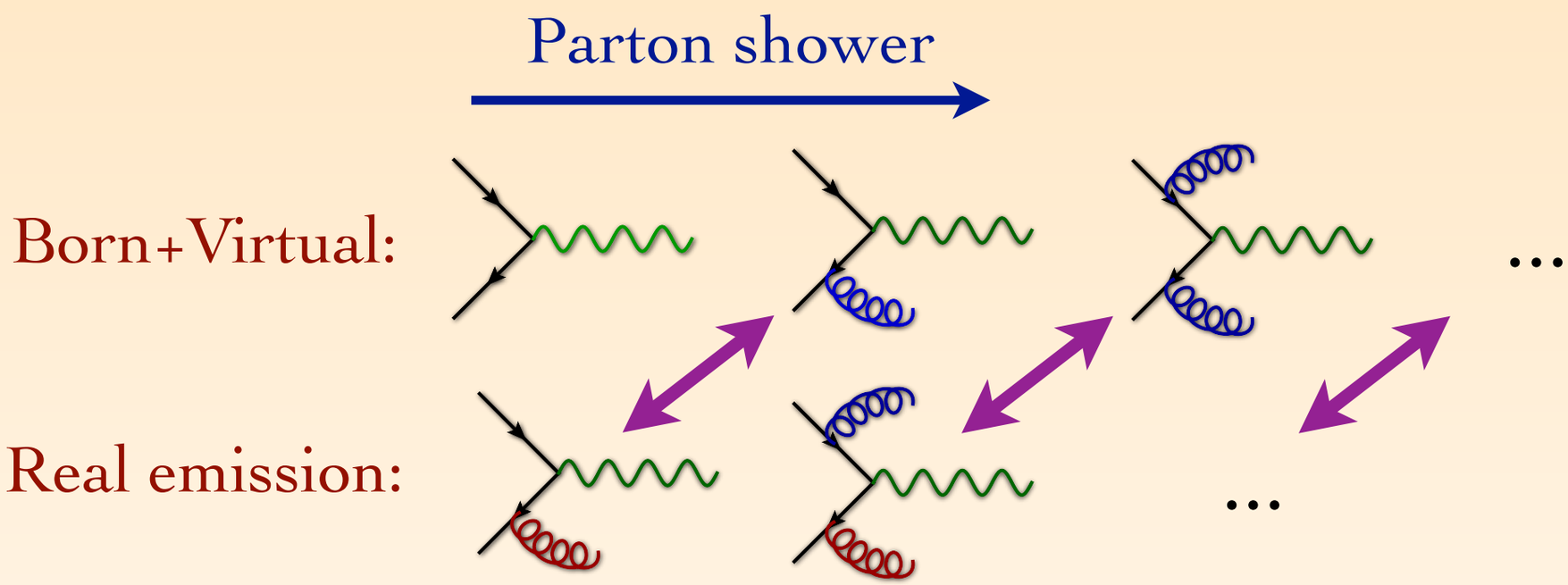


Sources of double counting



- 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 (Krakow group), Vincia (Skands et al.), …

MC@NLO procedure

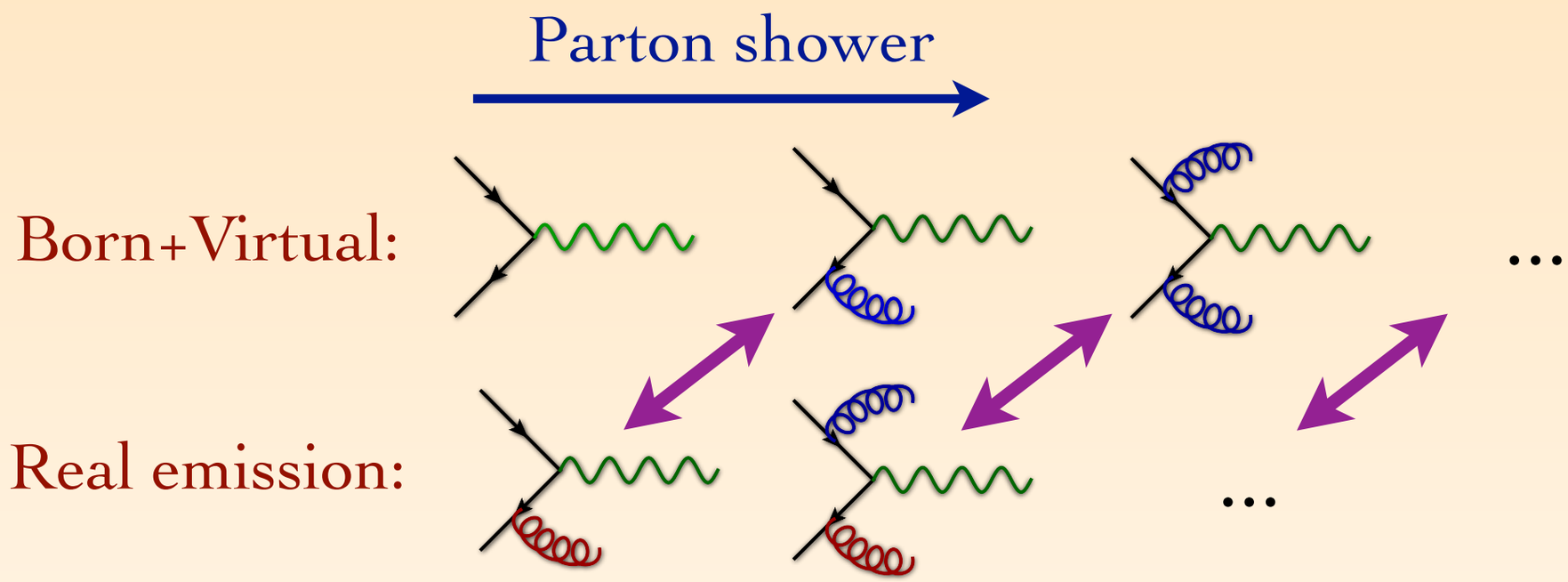
Frixione & Webber (2002)

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

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

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



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

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

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 (for the developer):

  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

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

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

Stability & unweighting

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

- 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 that I'll mention later

Negative weights

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

- 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 (i.e. making plots etc.)
- 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). Studies by Sherpa regarding this effect.
- **Fraction of negative weights can be large (30% negative weights is not rare)**
  - Requires larger samples of unweighted events to obtain the same statistical precision

POWHEG

Nason (2004)

- Consider the probability of the first emission of a leg (inclusive over later emissions). This is the usual patron shower starting from a Born event

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

- 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
  $$d\Phi_m\Big[B+V+\int d\Phi_1\, R\Big]\Big[1-\int d\Phi_1\frac{MC}{B}+d\Phi_1\frac{MC}{B}\Big]$$
  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:
  $$\Delta(Q^2,Q_0^2)=\exp\Big[-\int_{Q_0^2}^{Q^2}d\Phi_1\frac{MC}{B}\Big]\to\tilde{\Delta}(Q^2,Q_0^2)=\exp\Big[-\int_{Q_0^2}^{Q^2}d\Phi_1\frac{R}{B}\Big]$$
  corresponding to a modified differential branching probability
  $$d\tilde{p}=d\Phi_{(+1)}R/B$$

- Therefore we find for the POWHEG differential cross section
  $$d\sigma_{\text{powheg}}=d\Phi_m\Big[B+V+\int d\Phi_1 R\Big]\Big[\Delta(Q^2,Q_0^2)+\Delta(Q^2,t)d\Phi_1\frac{R}{B}\Big]$$

Properties

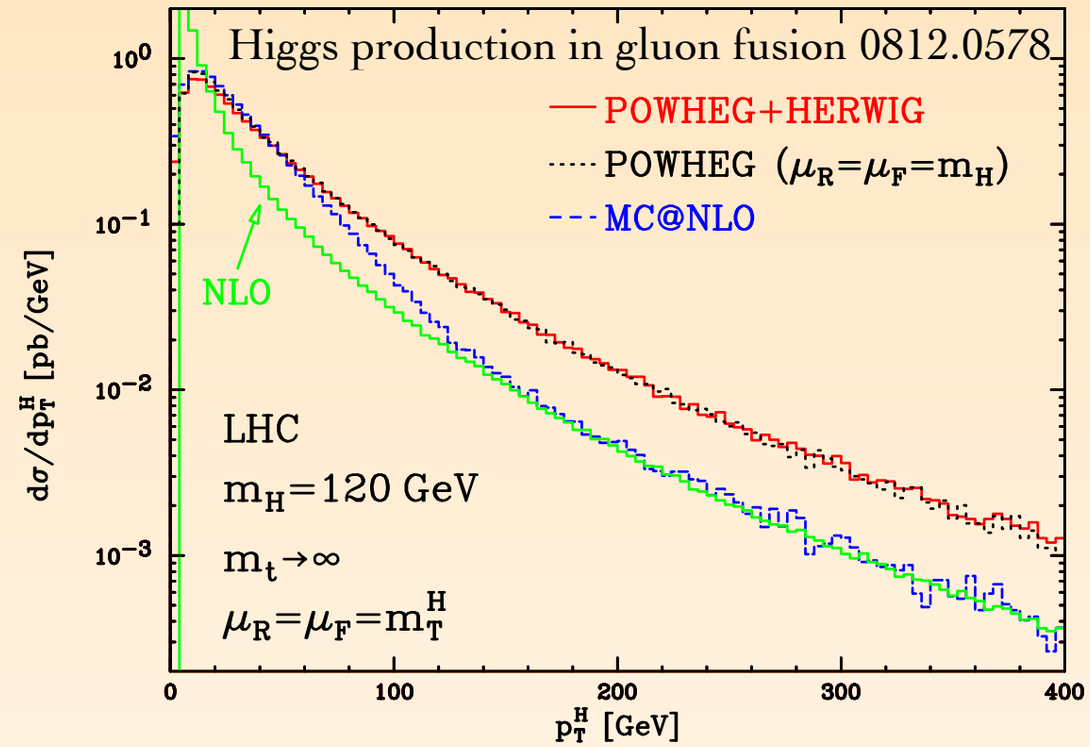
$$d\sigma_{\text{powheg}} = d\Phi_m \left[B + V + \int d\Phi_1 R \right] \left[\Delta(Q^2, Q_0^2) + \Delta(Q^2, t) d\Phi_1 \frac{R}{B} \right]$$

- 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



- ✦ NLO-factor multiples 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

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

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

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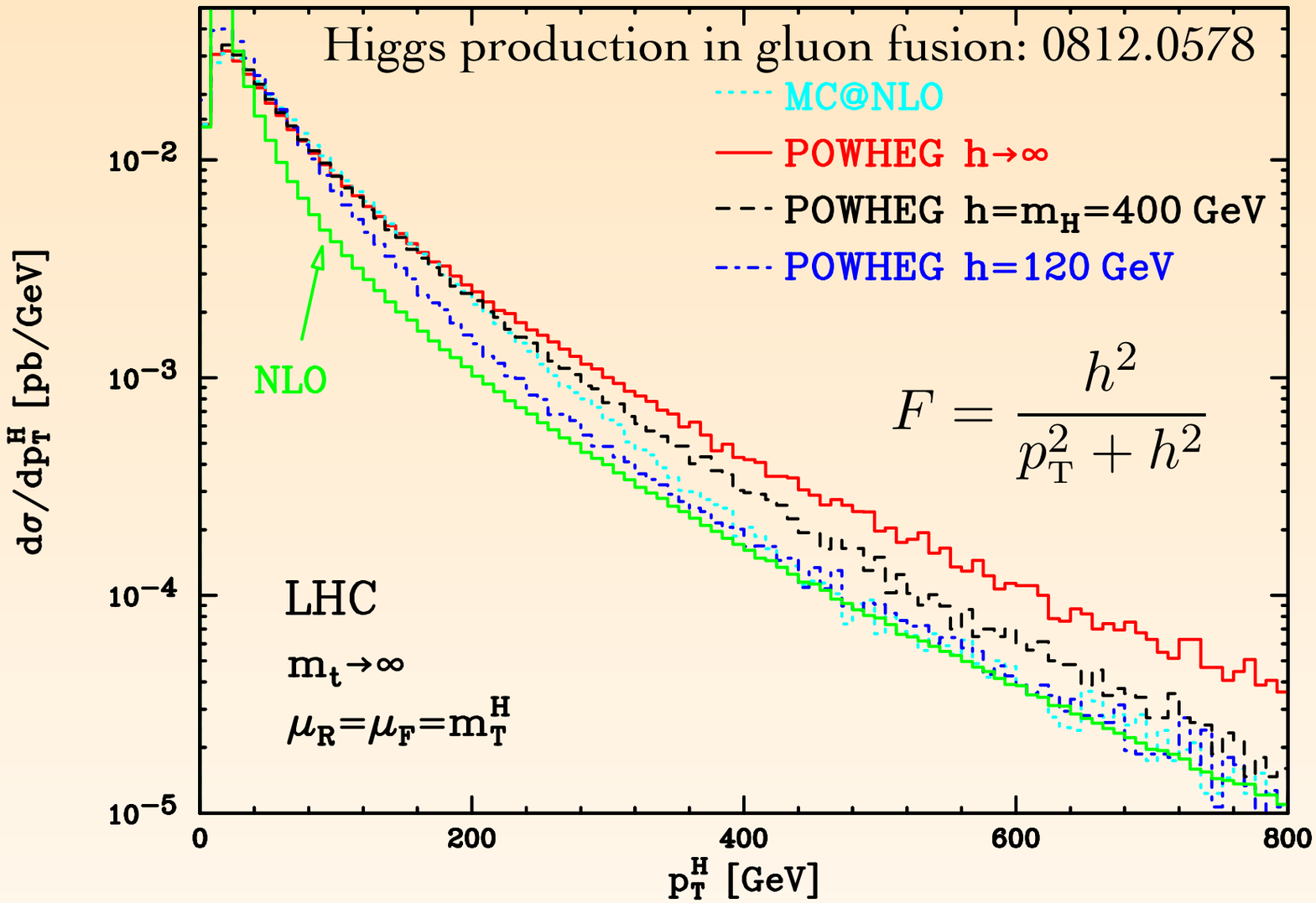
Original is F = 1 : exponentiate the full real; it can be damped by hand

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

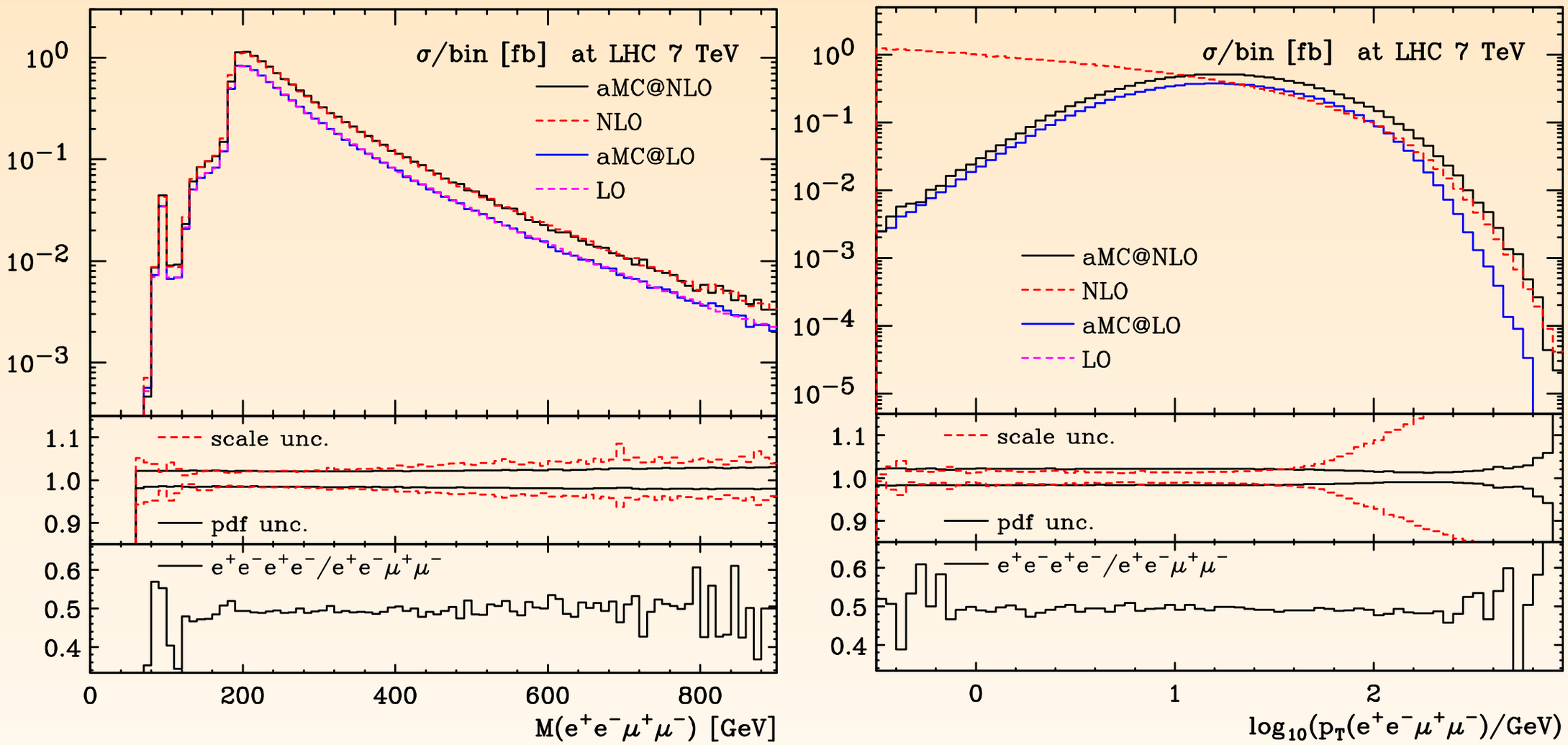
Damped POWHEG



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

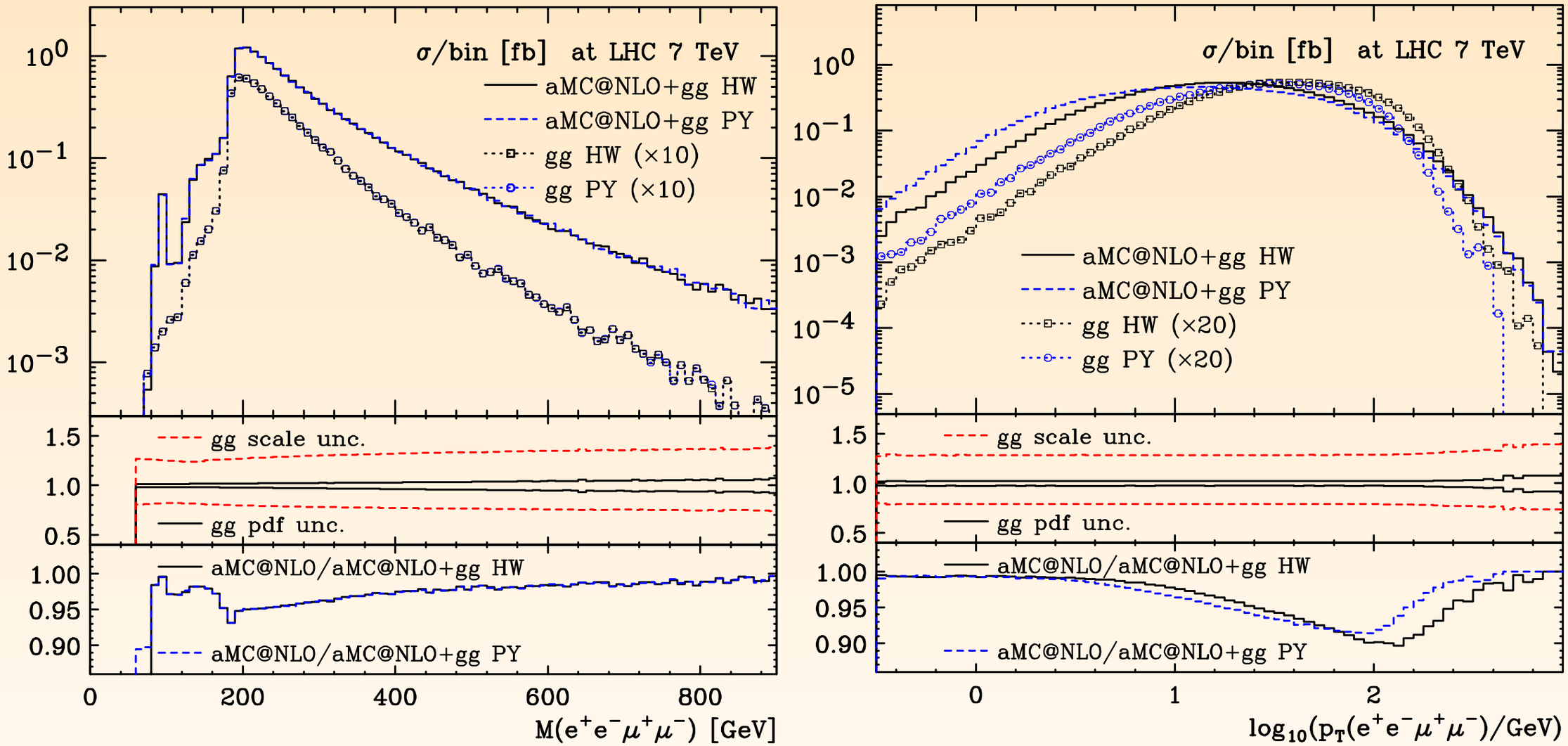
Four-lepton production

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

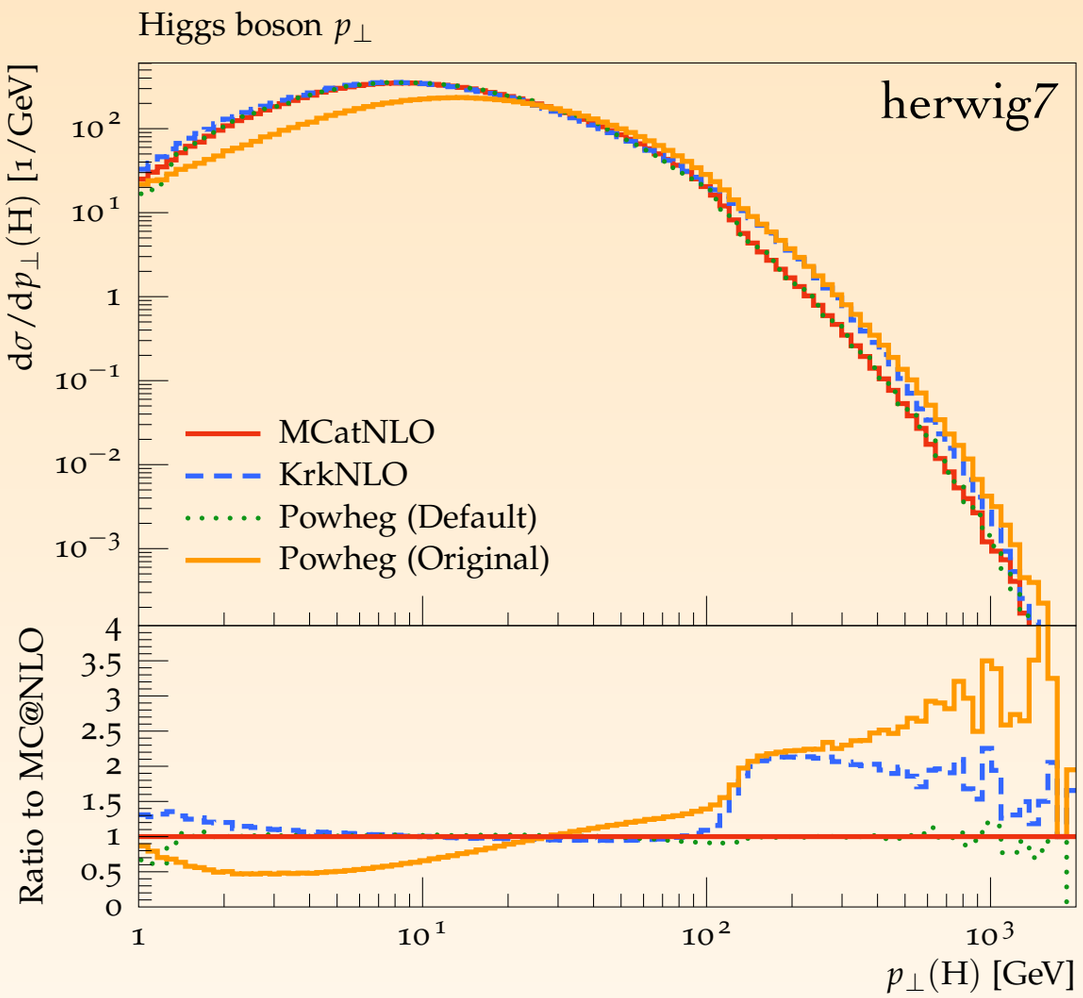
Four-lepton production

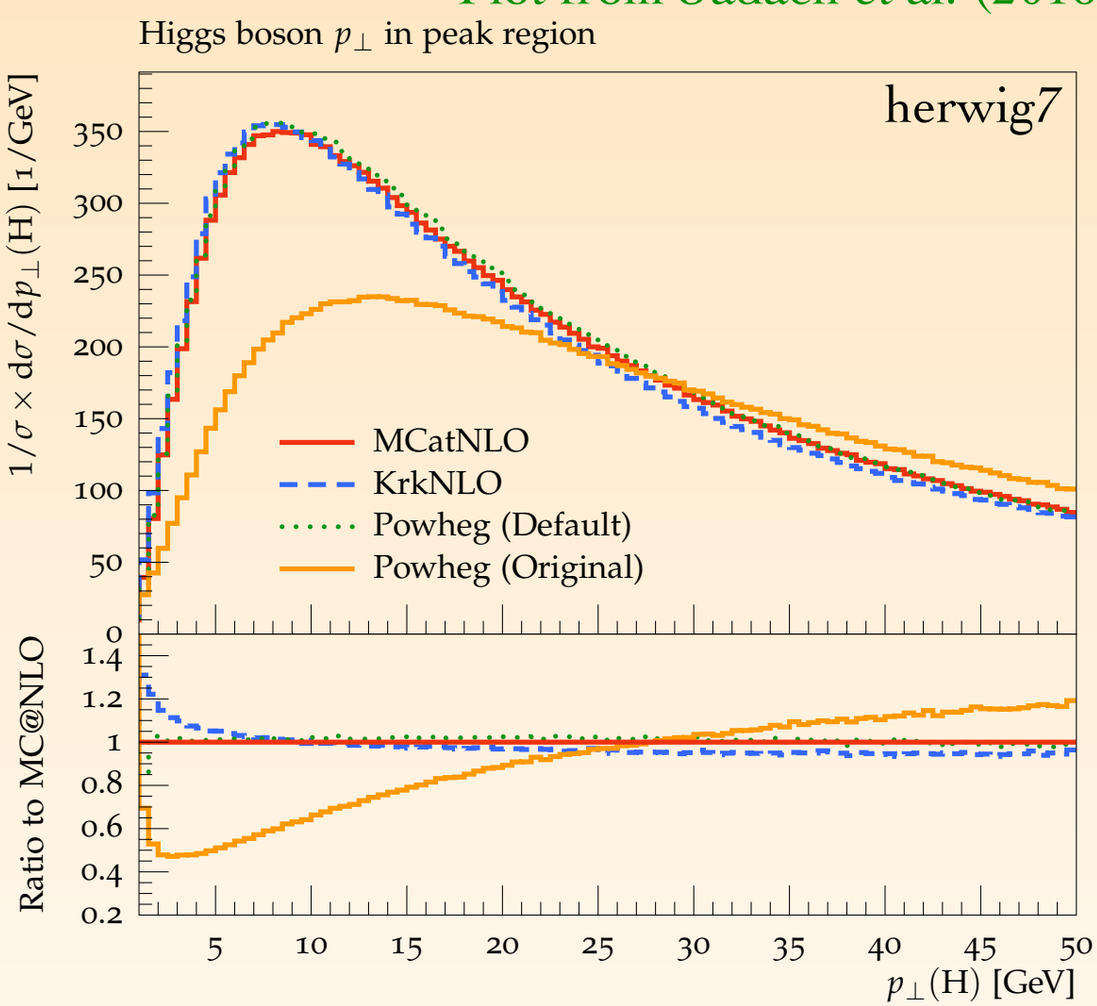


- Differences between Herwig (black) and Pythia (blue) showers large in the Sudakov suppressed region (much larger than the scale uncertainties)
- Contributions from gg initial state (formally NNLO) are of 5-10%

Higgs boson production

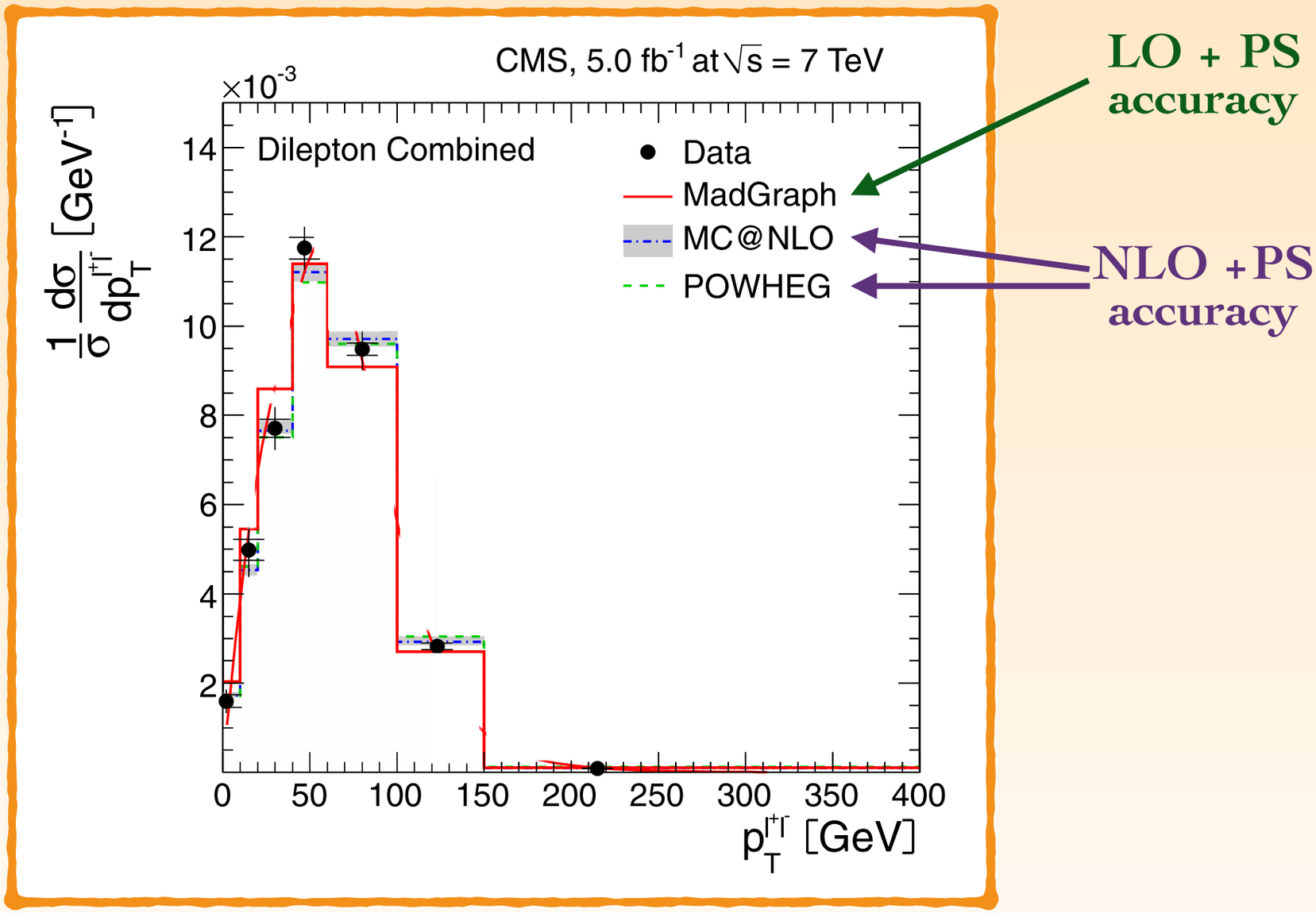
Plot from Jadach et al. (2016)





- Powheg: original: F=1, default F={1 for $p_T(H) < m_H$, 0 for $p_T(H) > m_H$}
  - Not only the tail is affected by the F parameter!
- KrkNLO method gets the hard tail without altering the small-p_T region

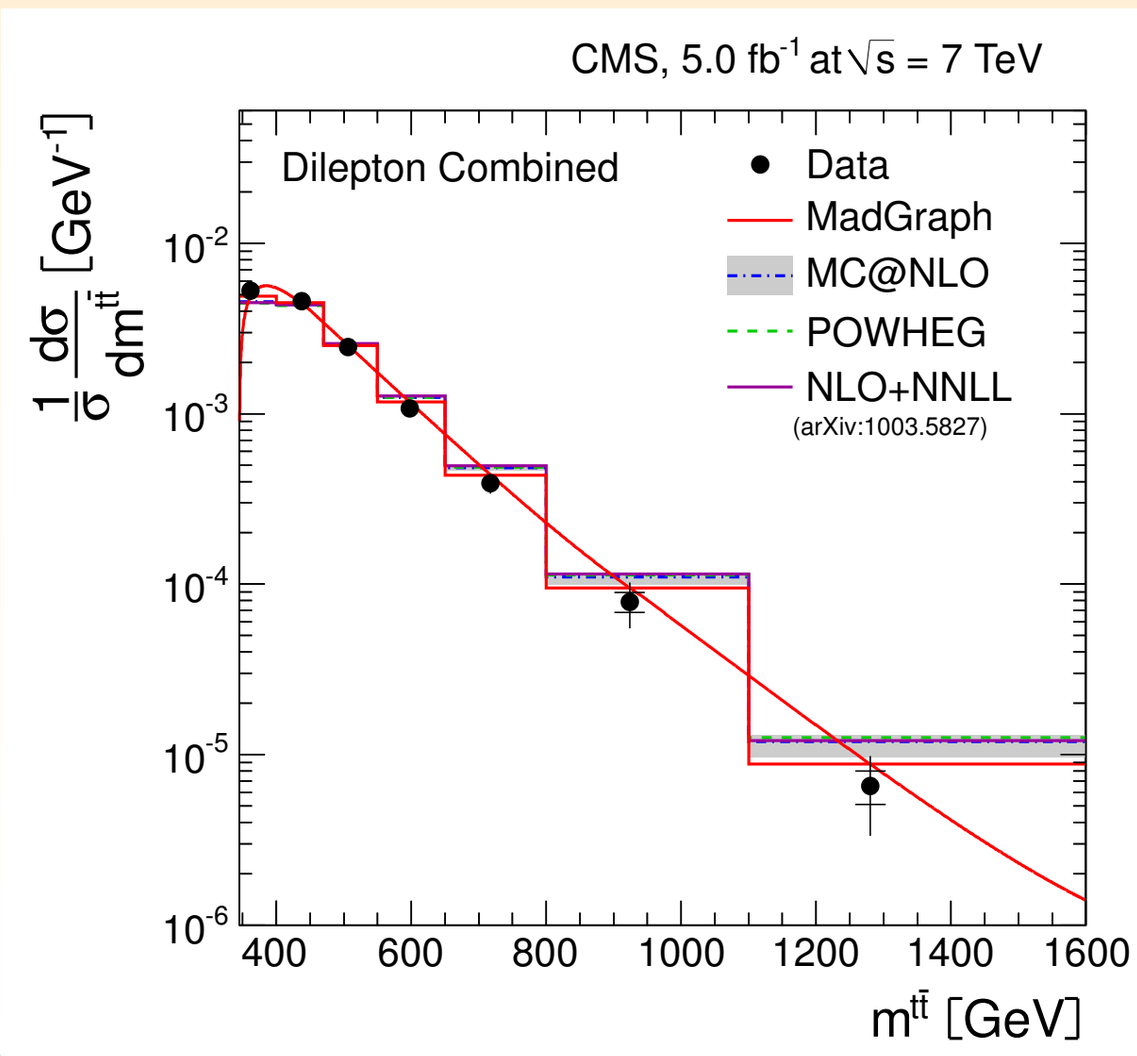
Quantitative predictions

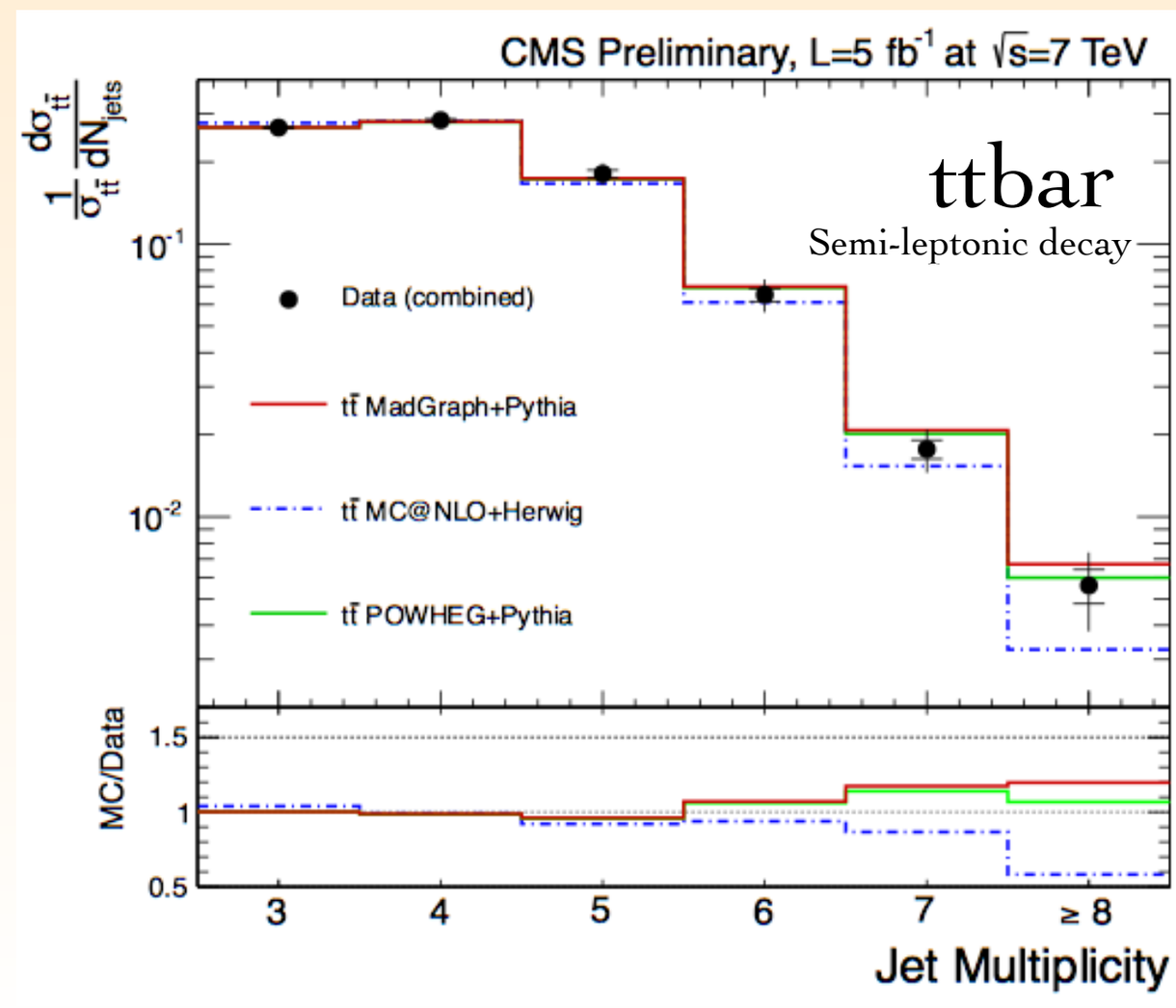


For precise, quantitative comparisons between theory and data, (at least) Next-to-Leading-Order corrections are a must

Is NLO+PS always the preferred method?

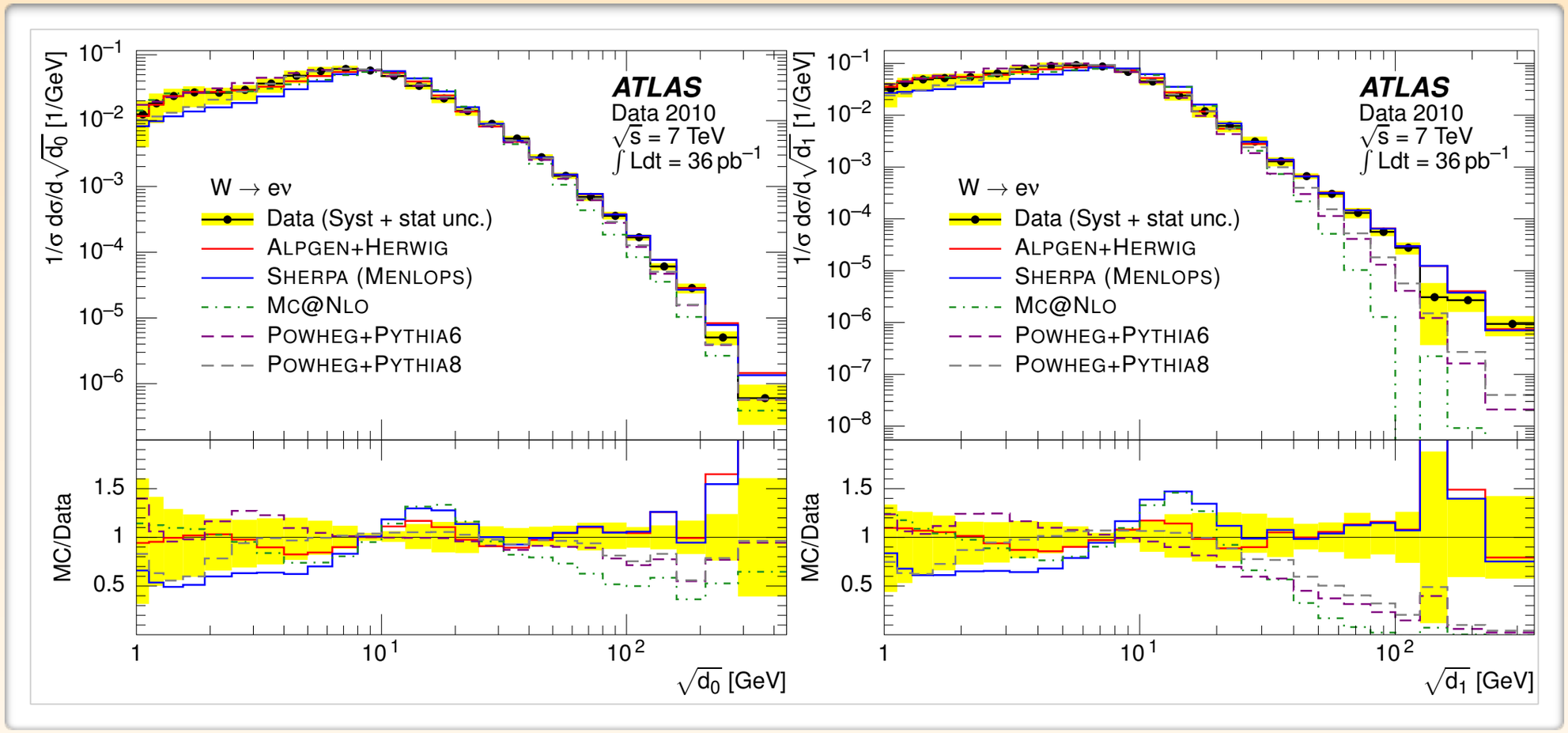
- It is the preferred method if the observable is described at NLO accuracy
- But there are many observables for which a given NLO+PS code has only zeroth order accuracy.





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