Introduction to Monte Carlo generators: Matching & Merging

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2024 CTEQ Summer School on QCD and Electroweak Phenomenology,
Hosted by the University of Münster, Germany

An LHC collision, factorised

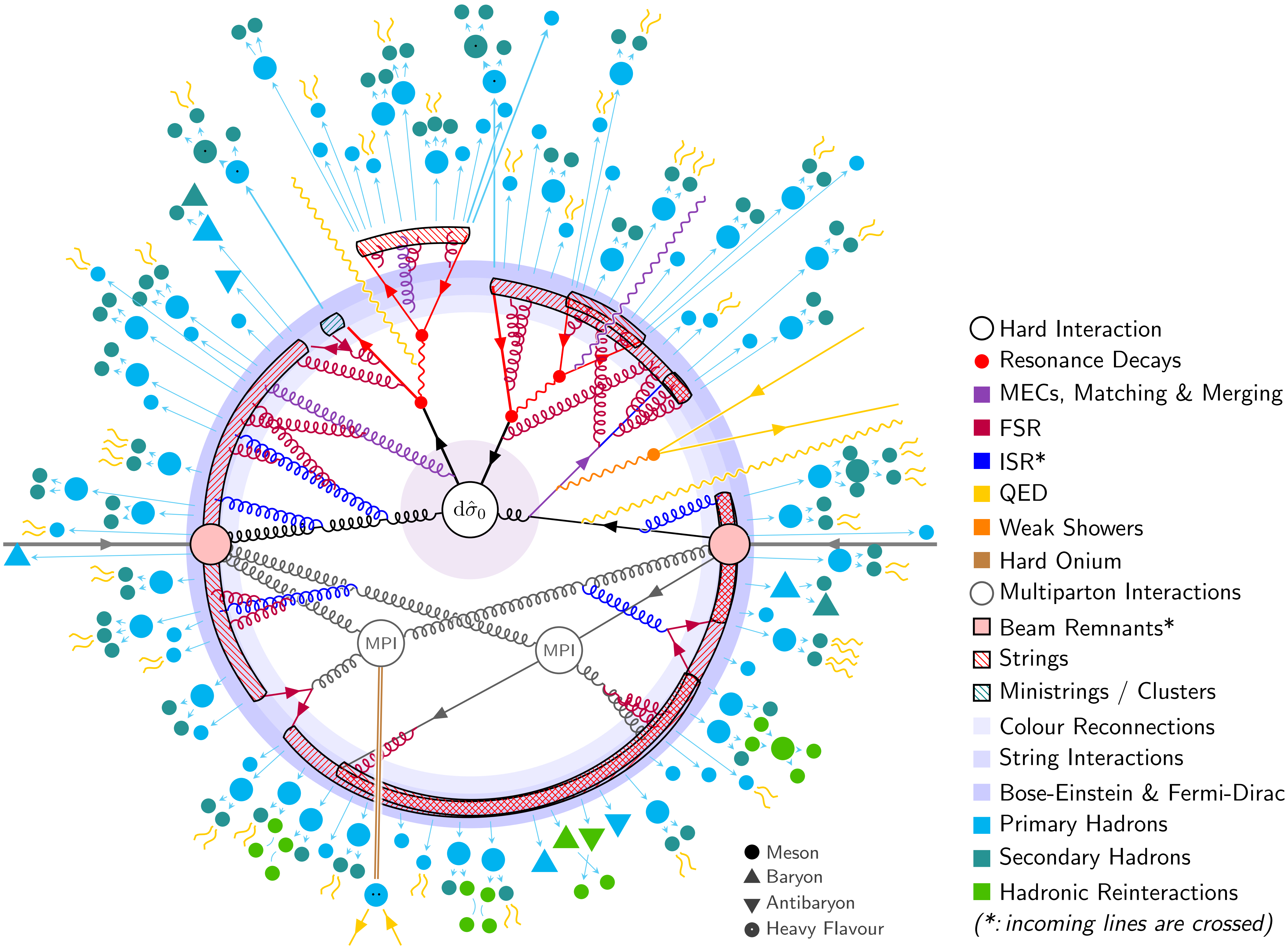
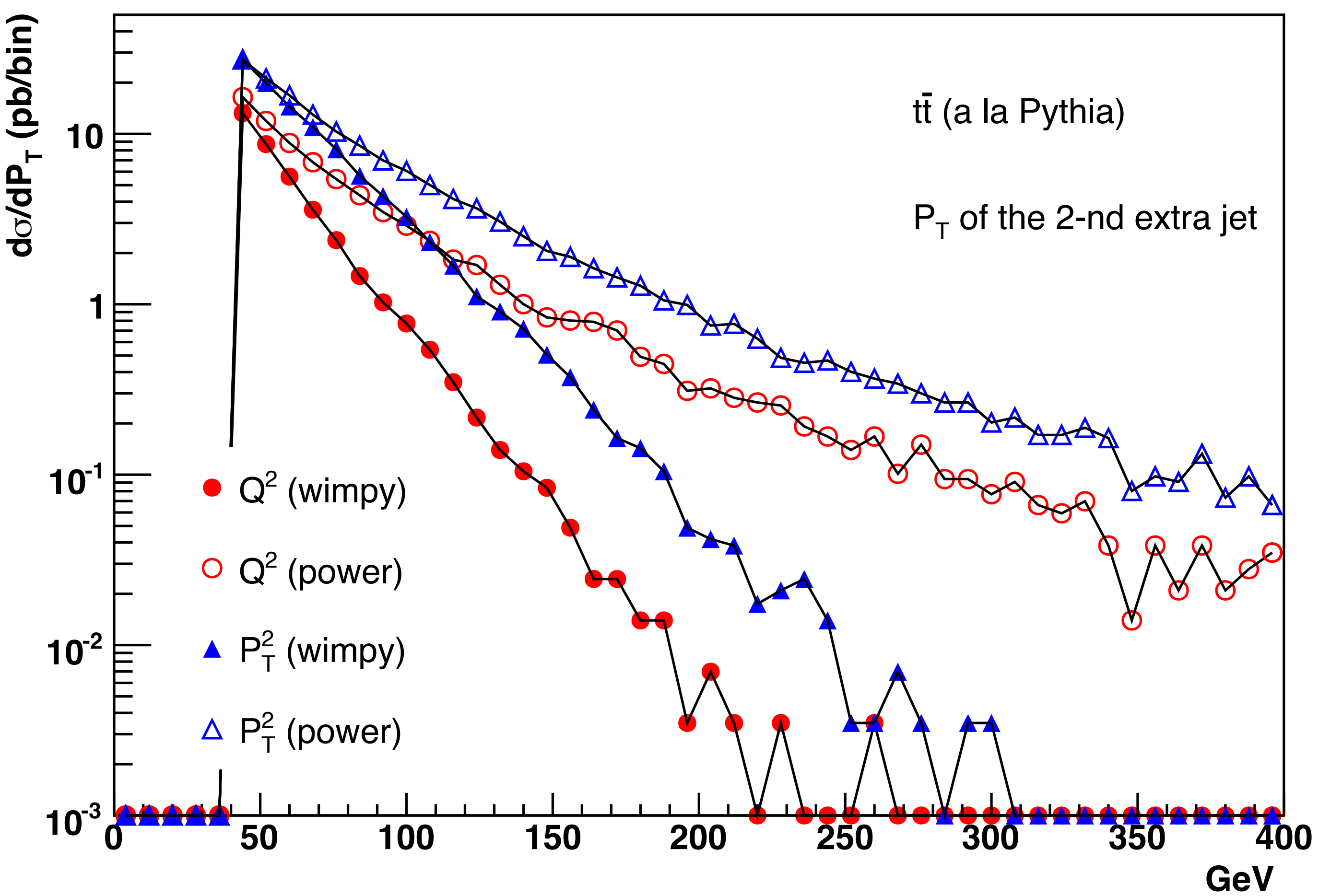


Figure taken from Bierlich et al., 2022 *(Pythia8.3 manual)*

Improving Parton Showers
LO merging

Collinear approximation

- The parton shower is correct in the collinear limit
  - But we use it also outside of this limit
  - Induces great dependence on the details of the implementation



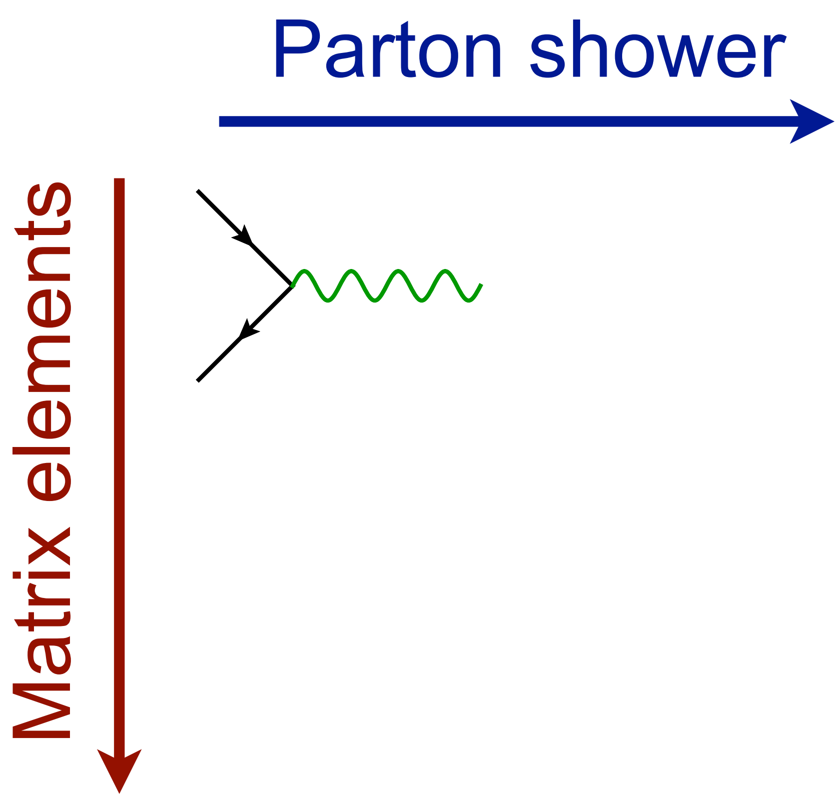
Matrix elements vs. Parton showers

ME	Shower MC
1. Fixed order calculation	1. Resums logs to all orders
2. Computationally expensive	2. Computationally cheap
3. Limited number of particles	3. No limit on particle multiplicity
4. Valid when partons are hard and well separated	4. Valid when partons are collinear and/or soft
5. Quantum interference correct	5. Partial interference through angular ordering
6. Needed for multi-jet description	6. Needed for hadronisation

Approaches are complementary: merge them!

Avoid double counting, ensure smooth distributions

Possible double counting



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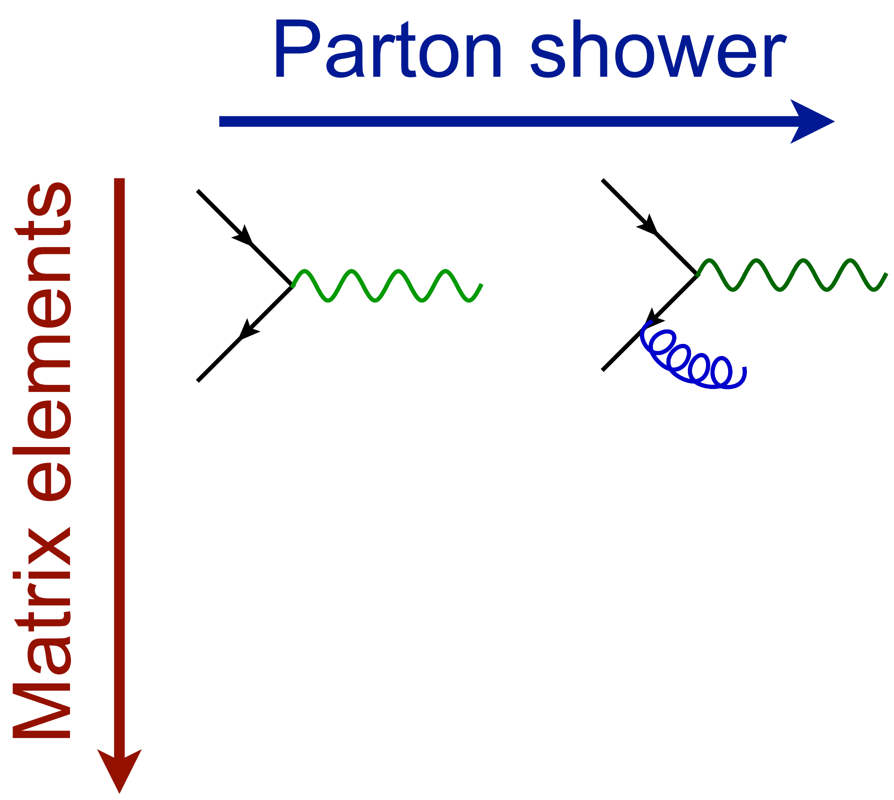

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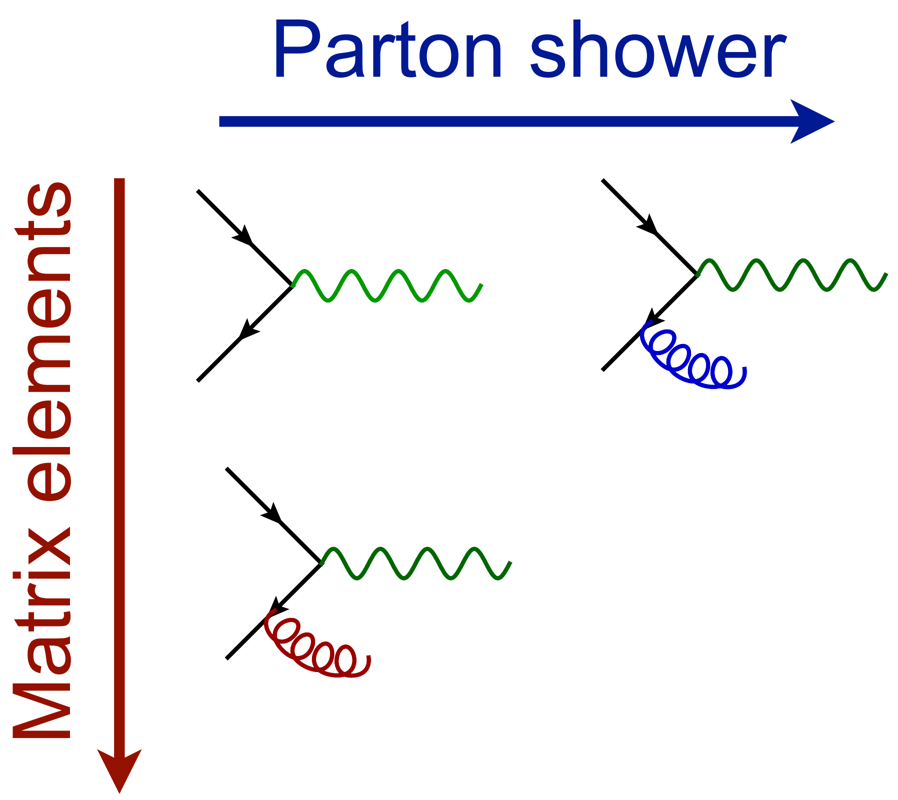

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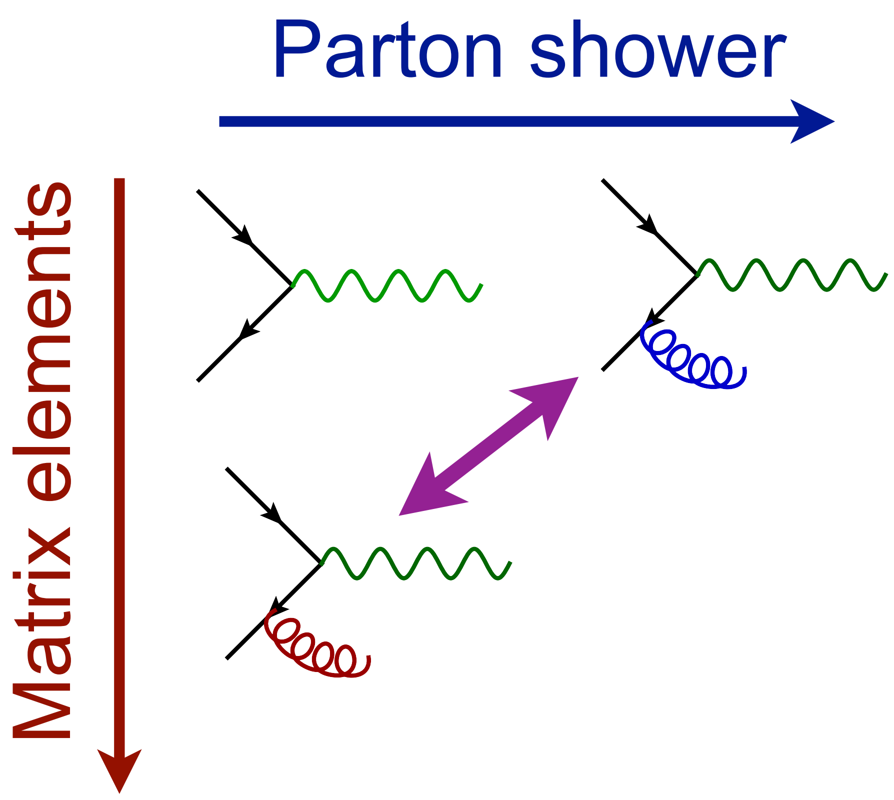

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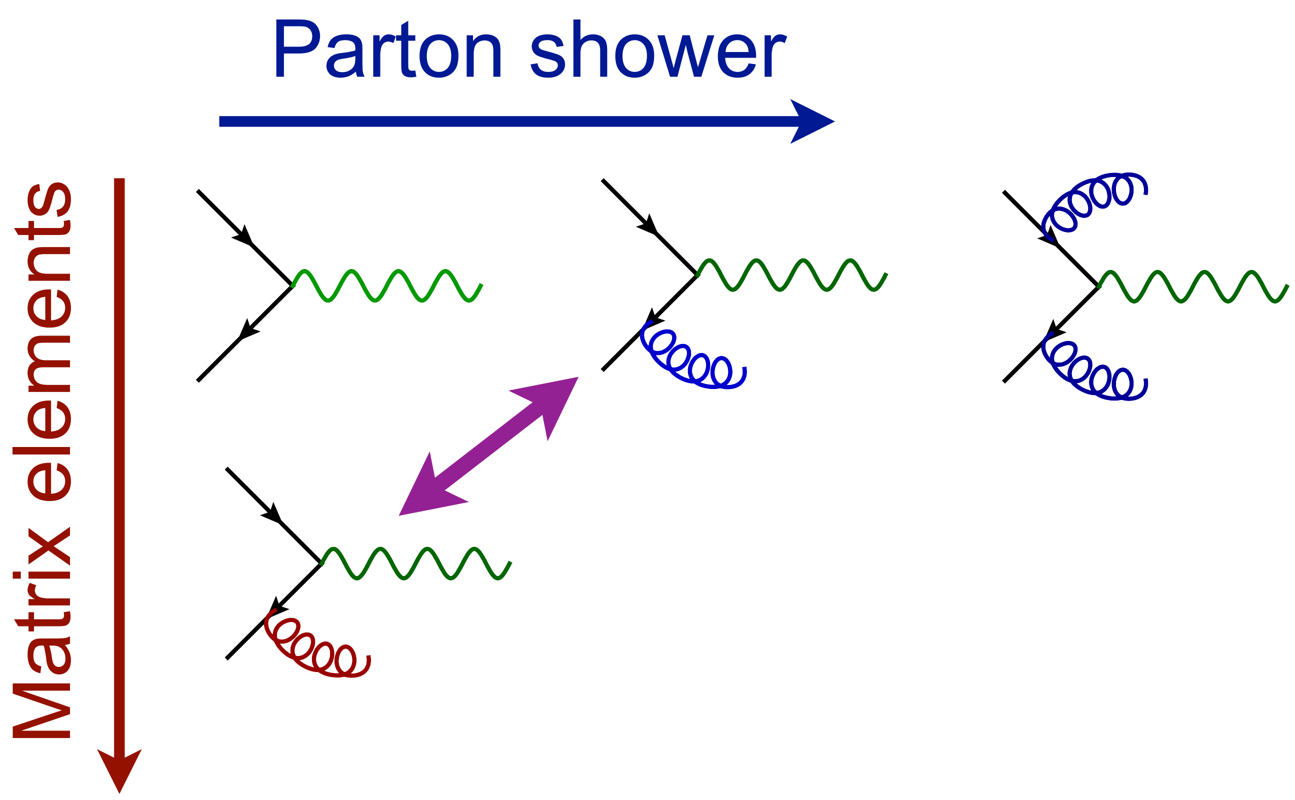

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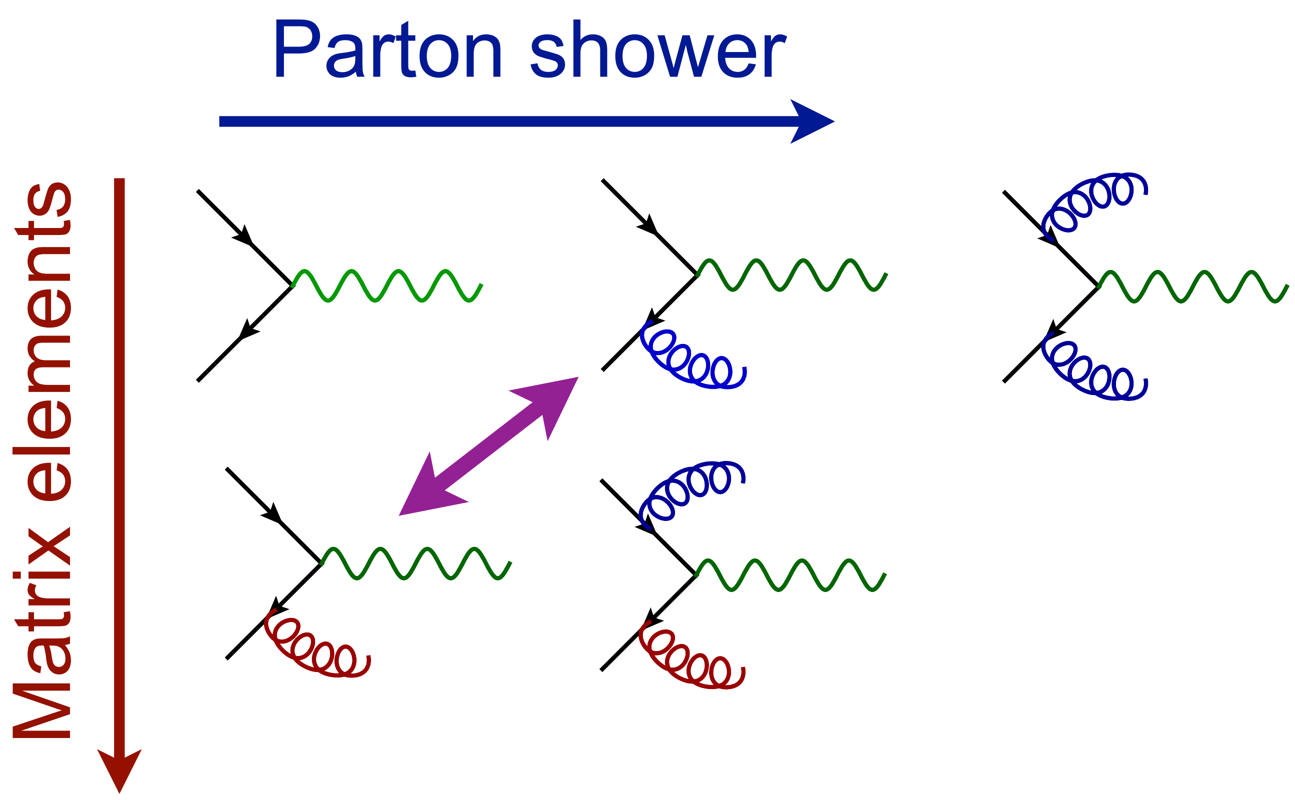

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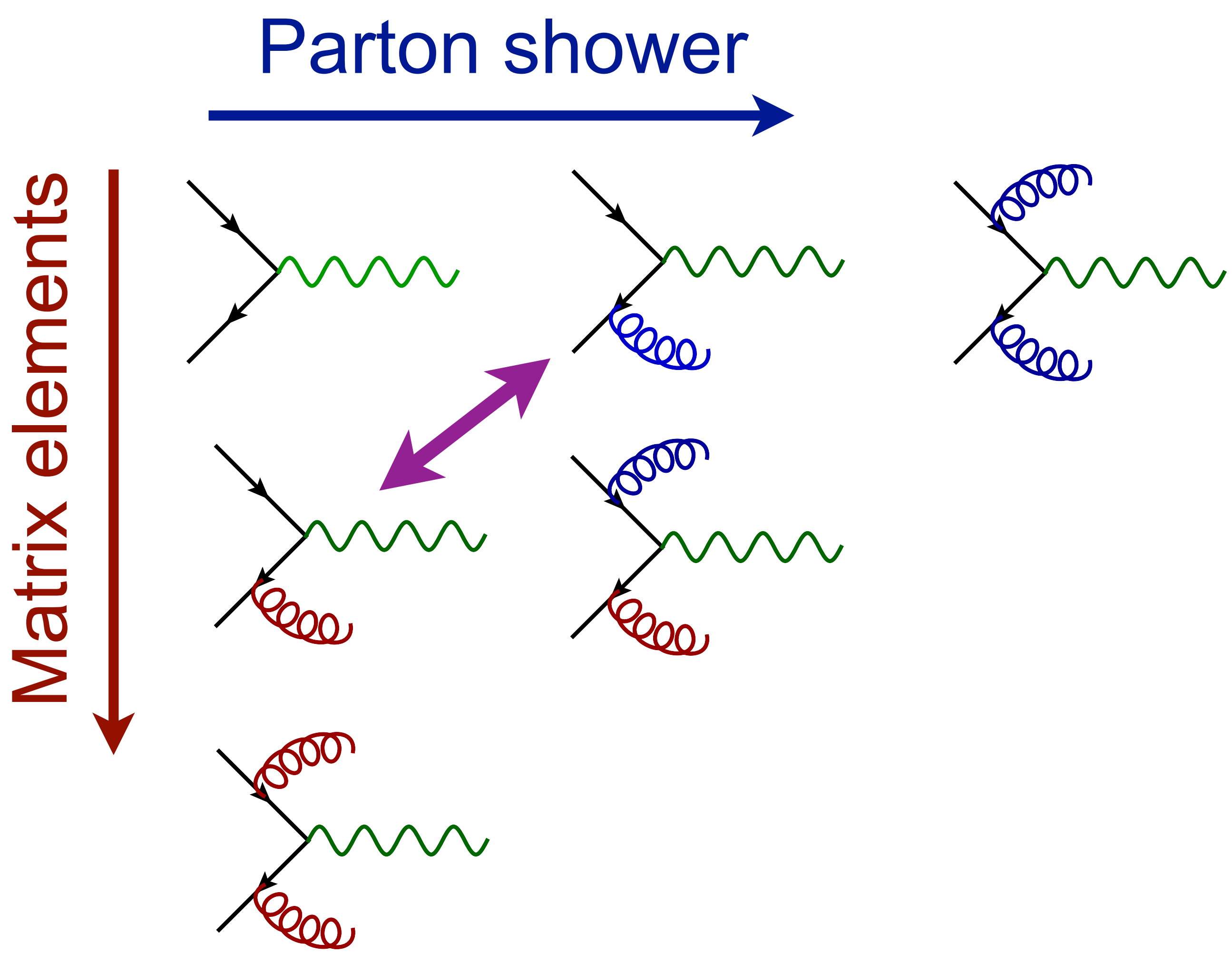

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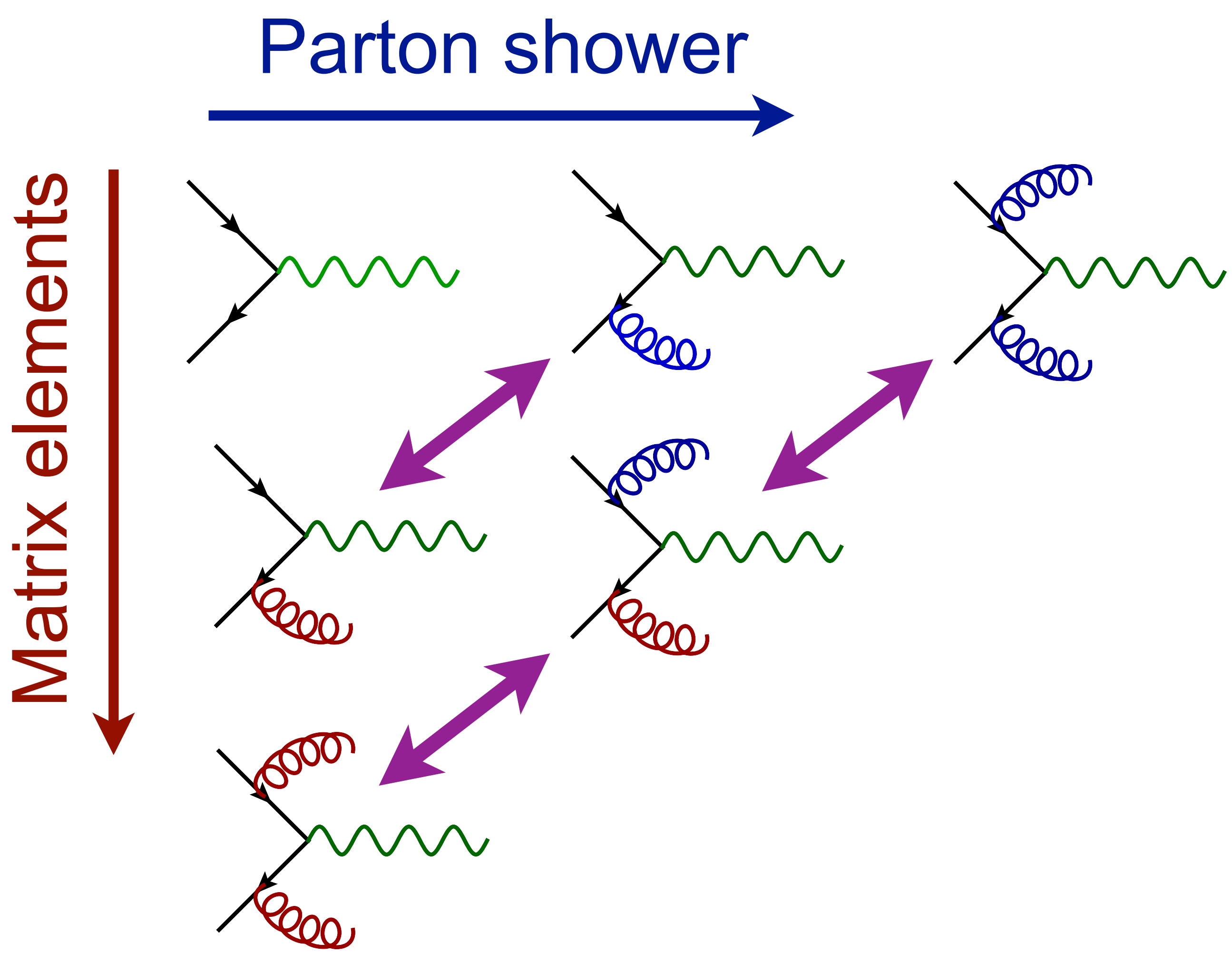

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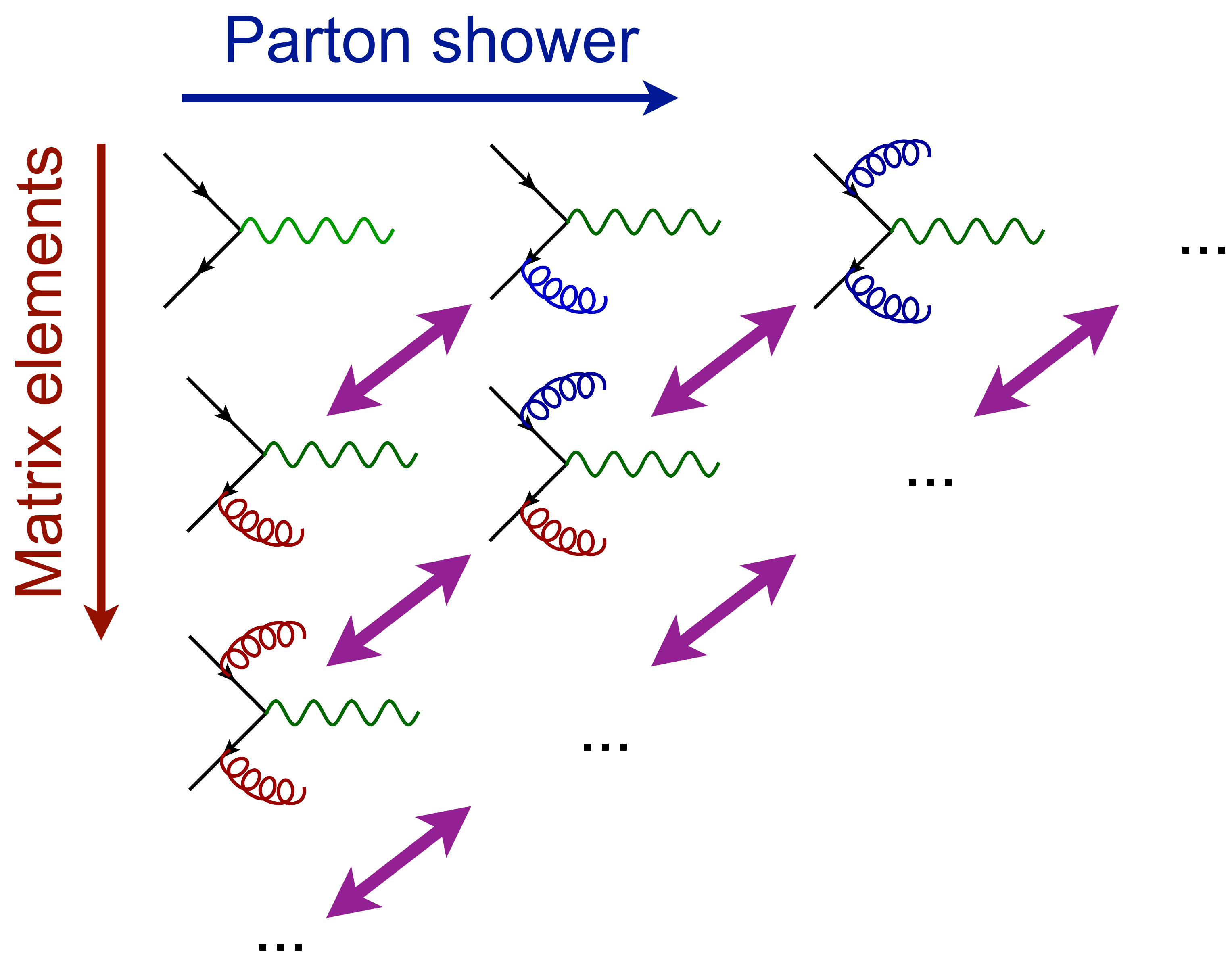

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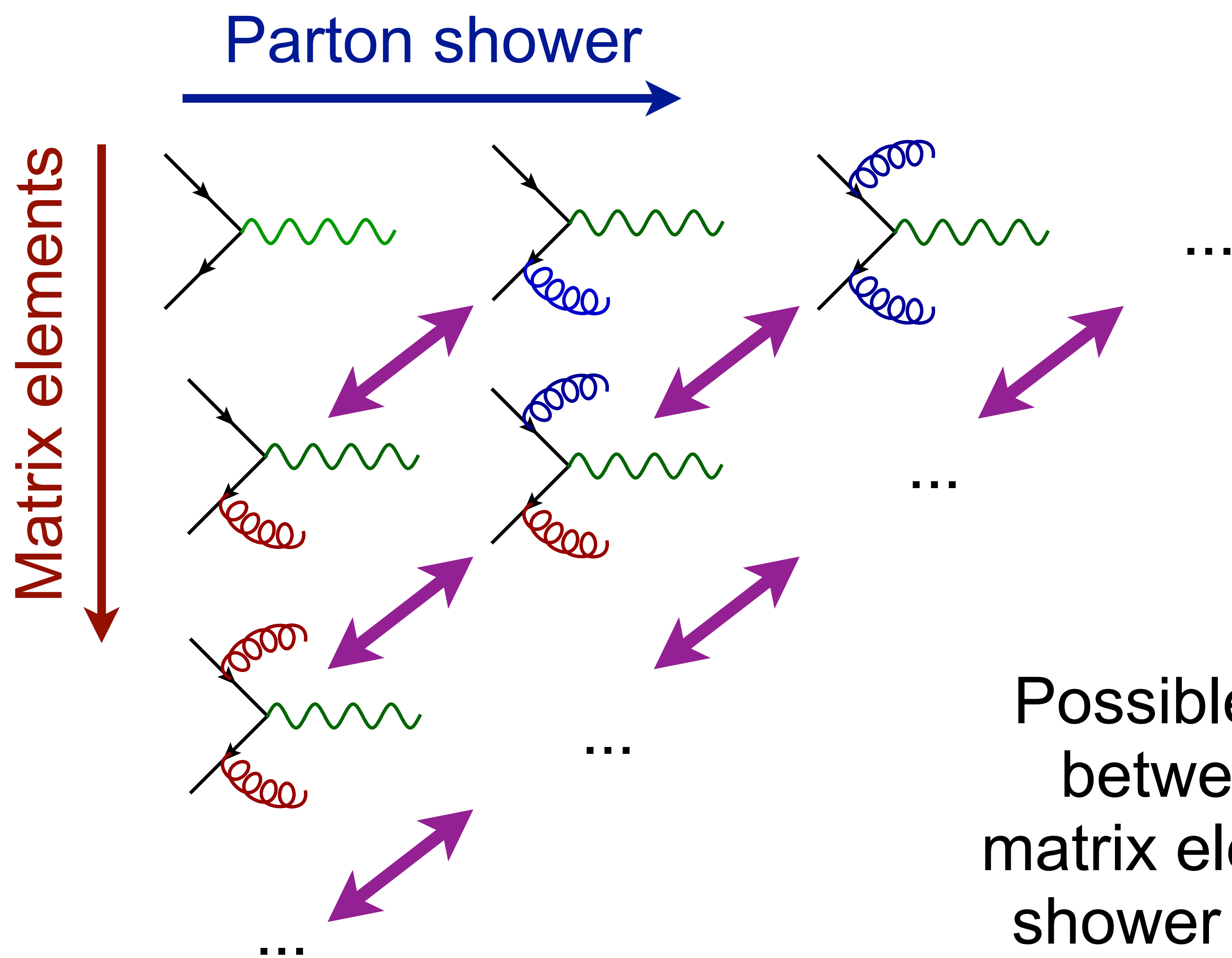

Possible double counting between partons from matrix elements and parton shower easily avoided by applying a cut in phase space

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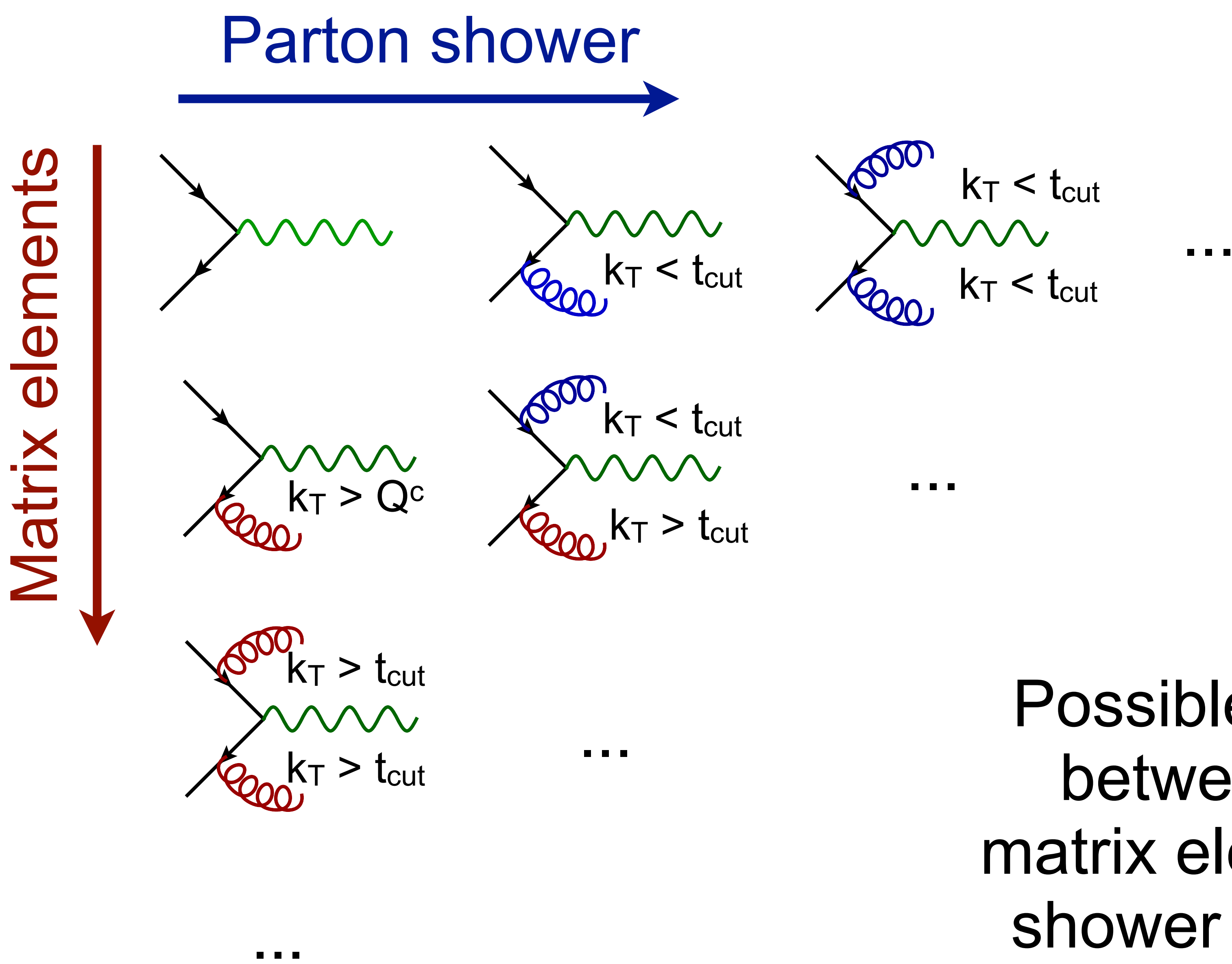
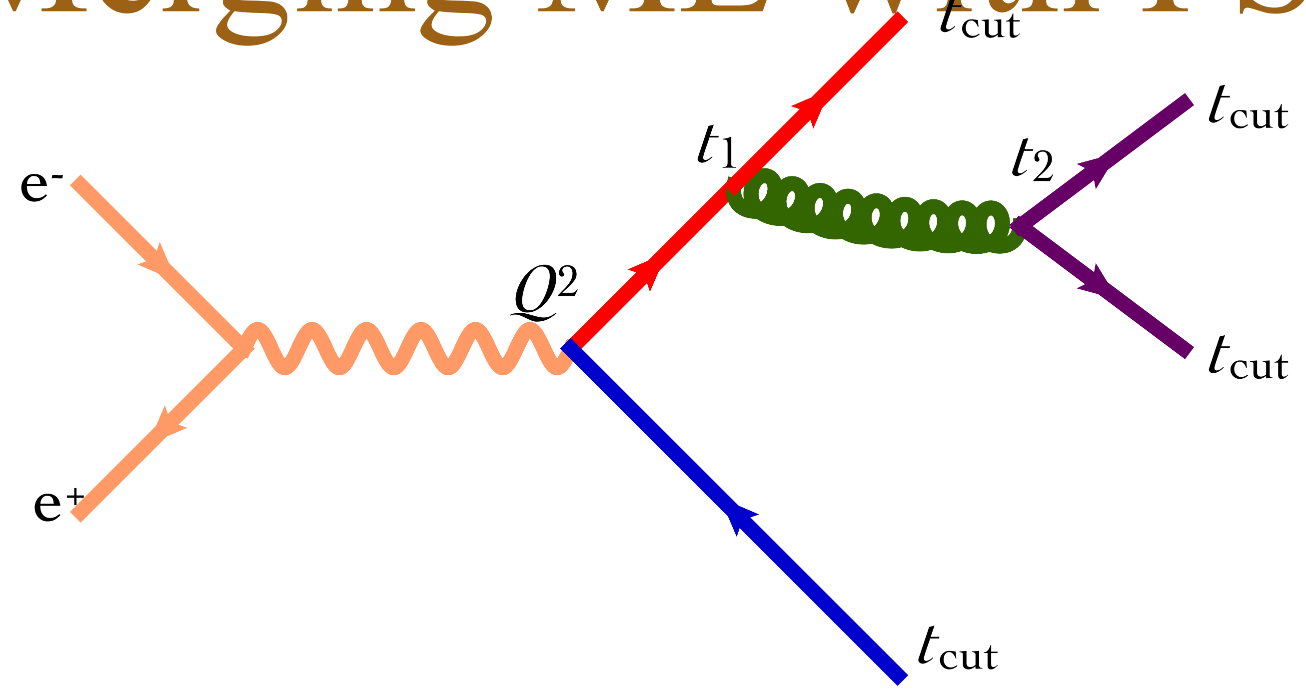


Possible double counting between partons from matrix elements and parton shower easily avoided by applying a cut in phase space

Merging ME with PS

- So double counting no problem, but what about getting smooth distributions that are independent of the precise value of t_{cut}?
- 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

$$(\Delta_q(Q^2, t_{\rm cut}))^2 \Delta_g(t_1, t_2)(\Delta_q(t_2, t_{\rm cut}))^2 \frac{\alpha_s(t_1)}{2\pi} P_{gq}(z) \frac{\alpha_s(t_2)}{2\pi} P_{qg}(z')$$

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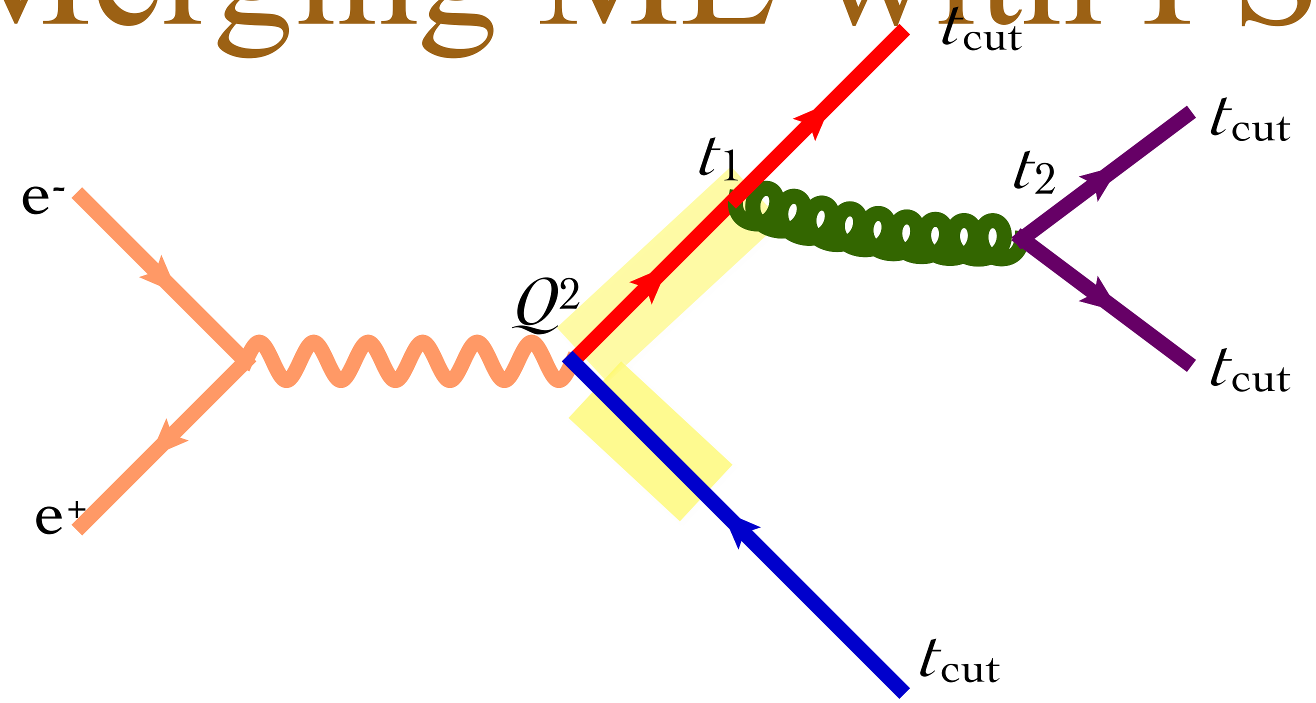

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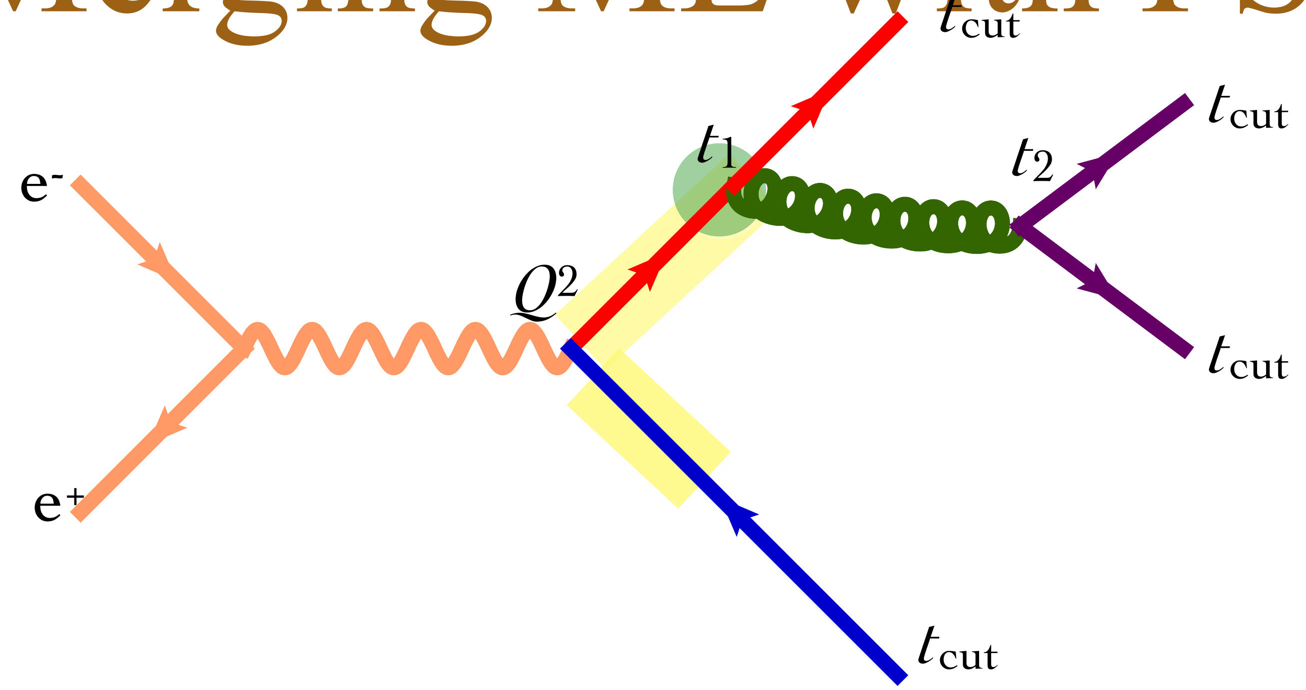

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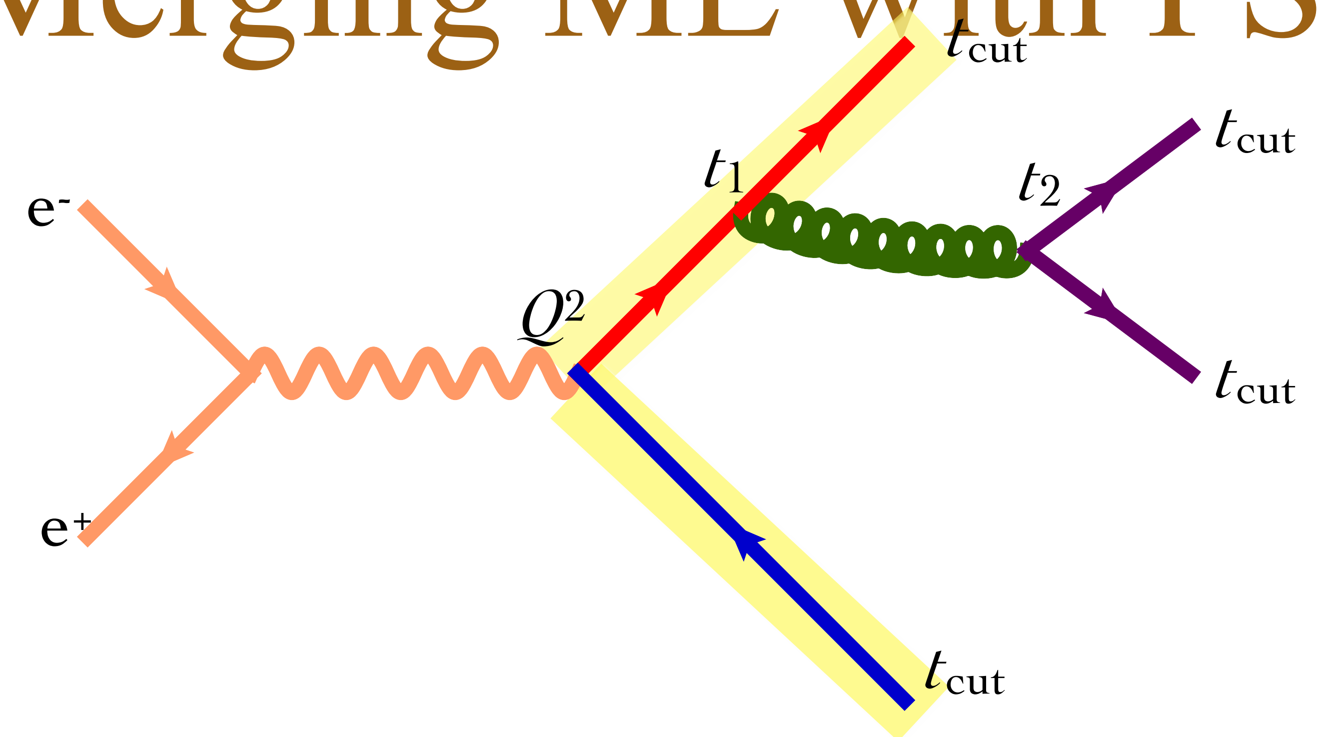

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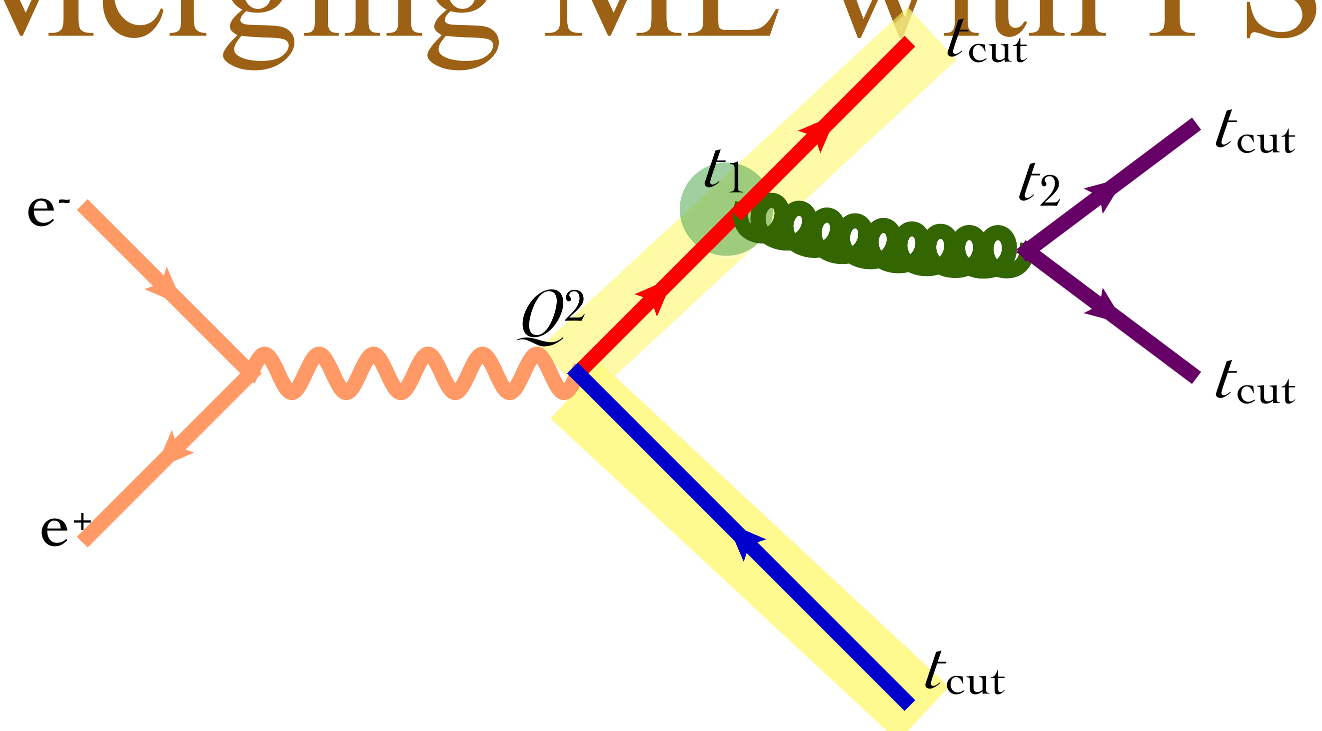

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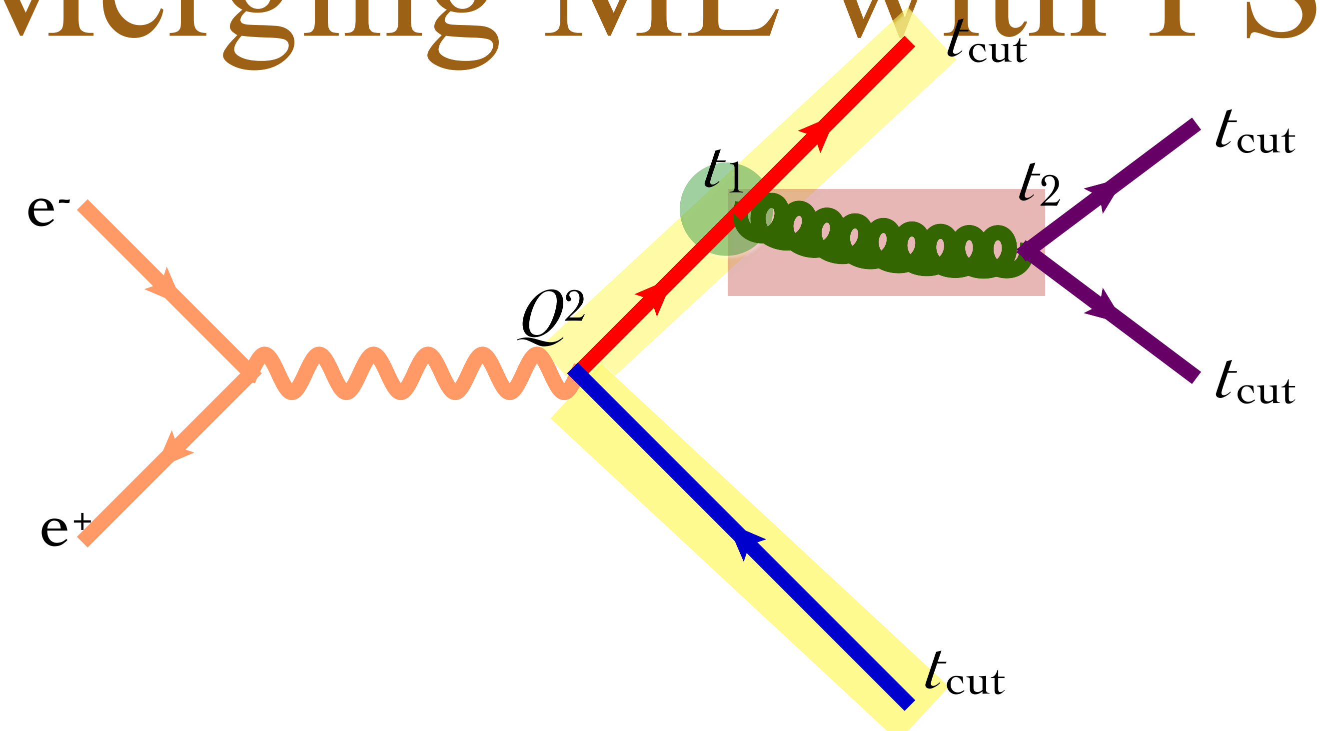

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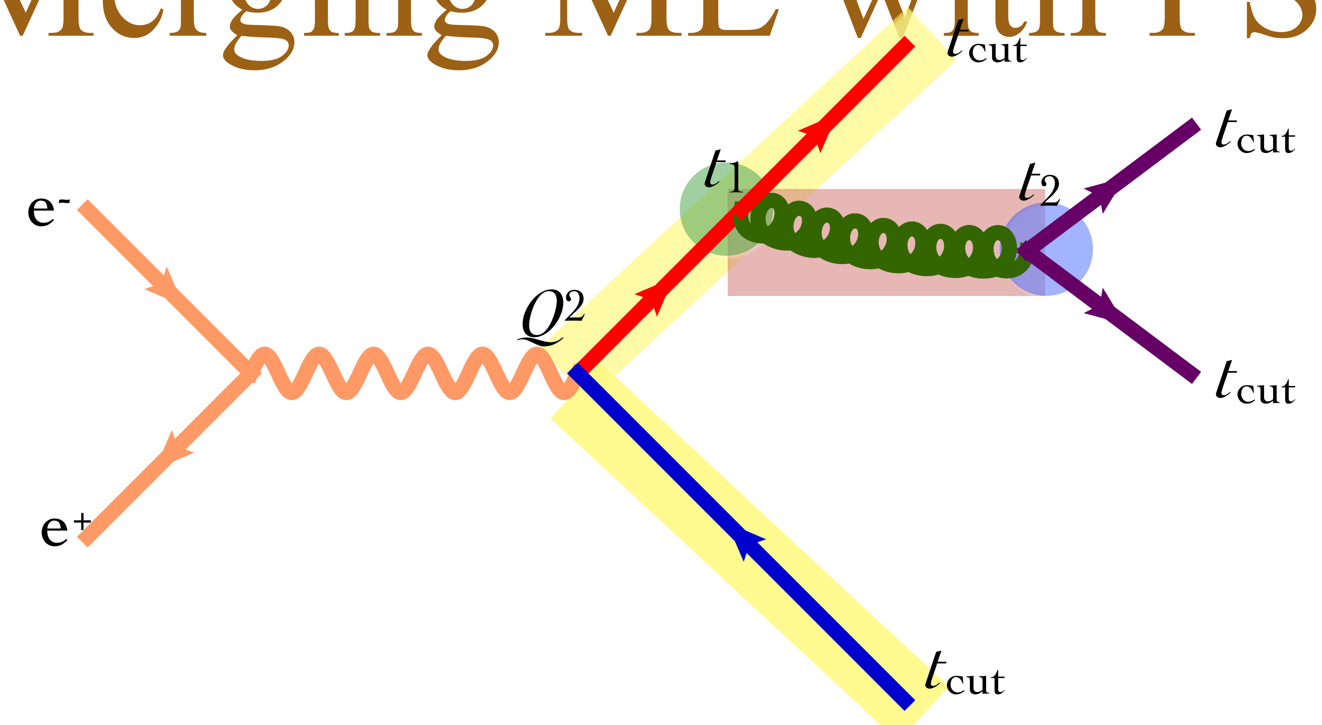

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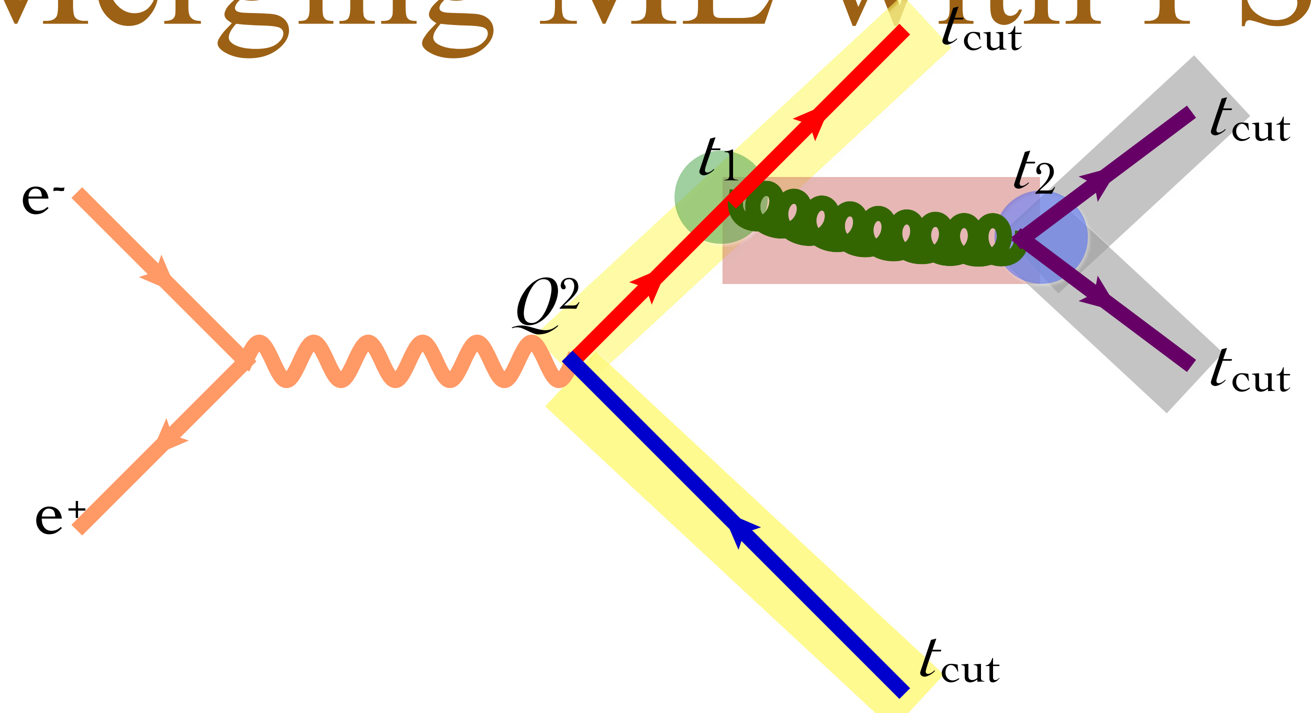

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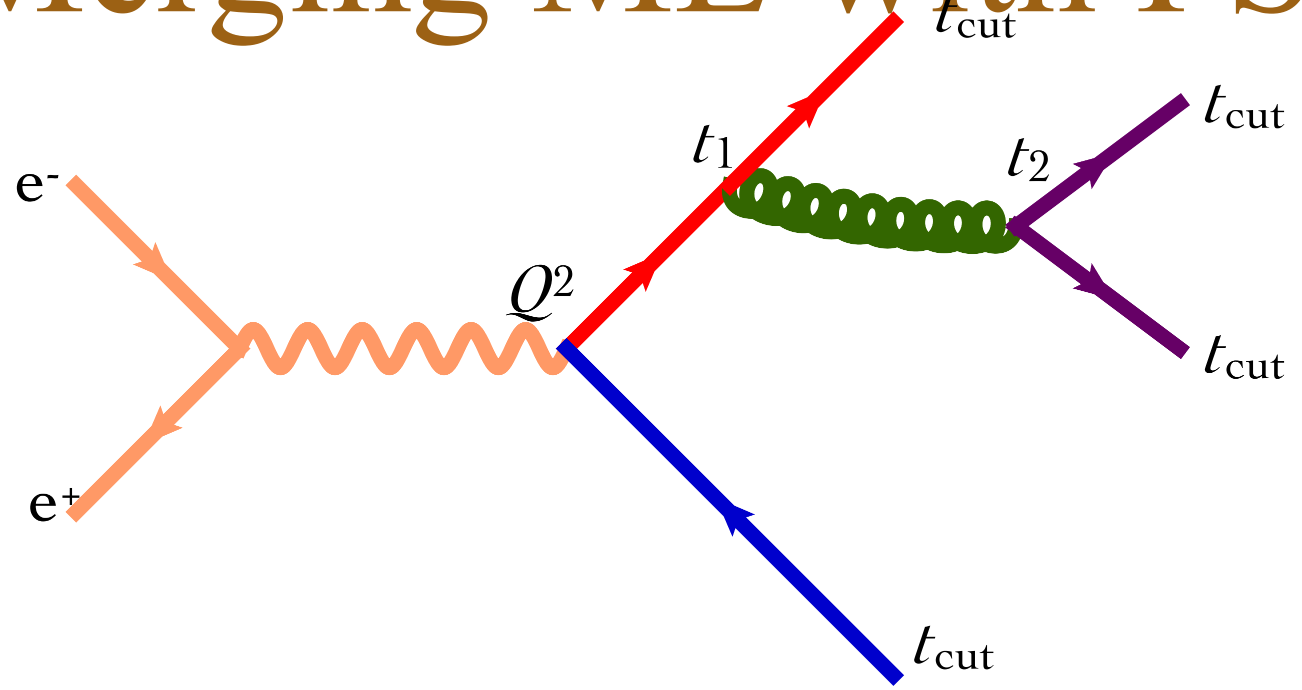

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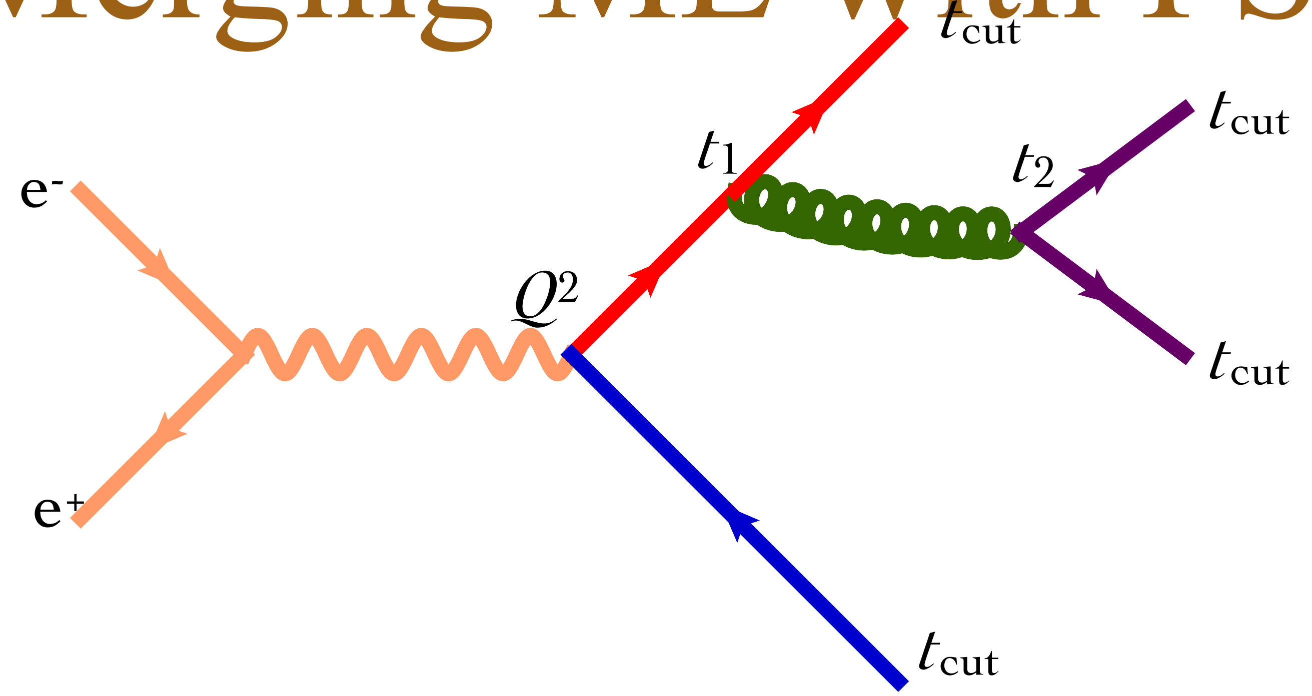

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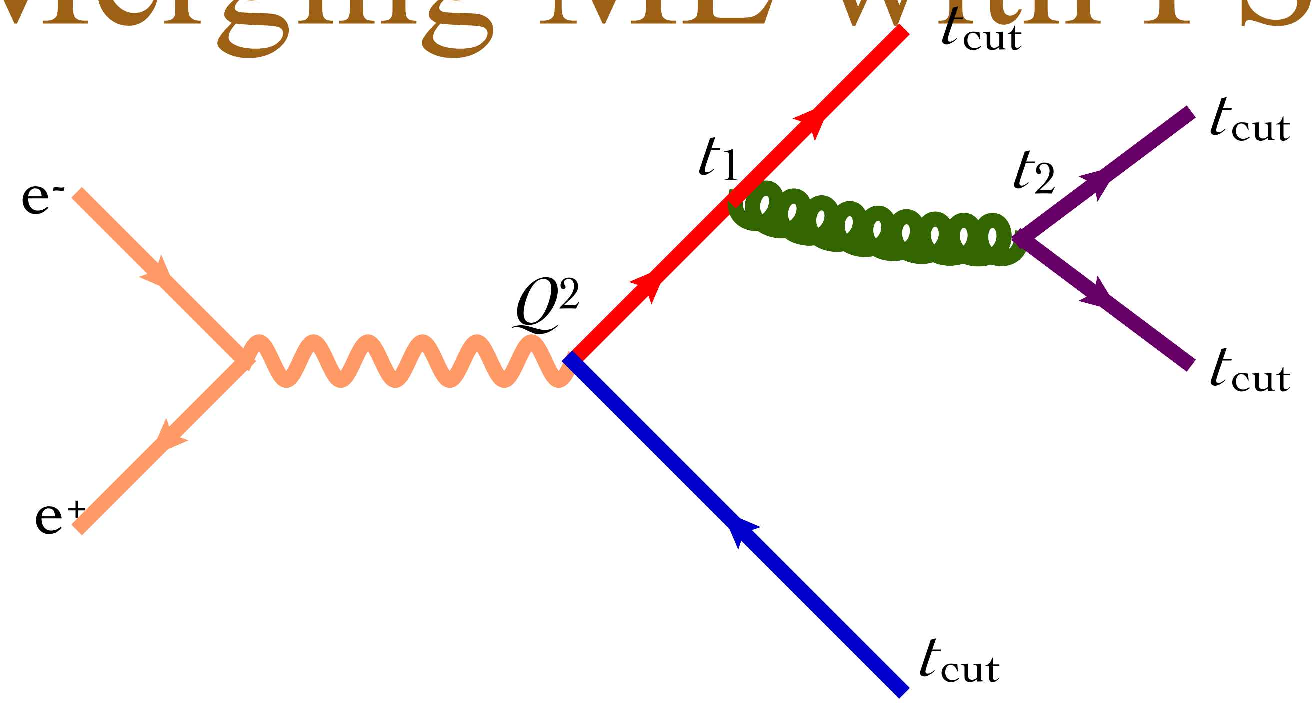
Leading Logarithmic approximation of the matrix element
BUT with α_s evaluated at the scale of each splitting

Merging ME with PS



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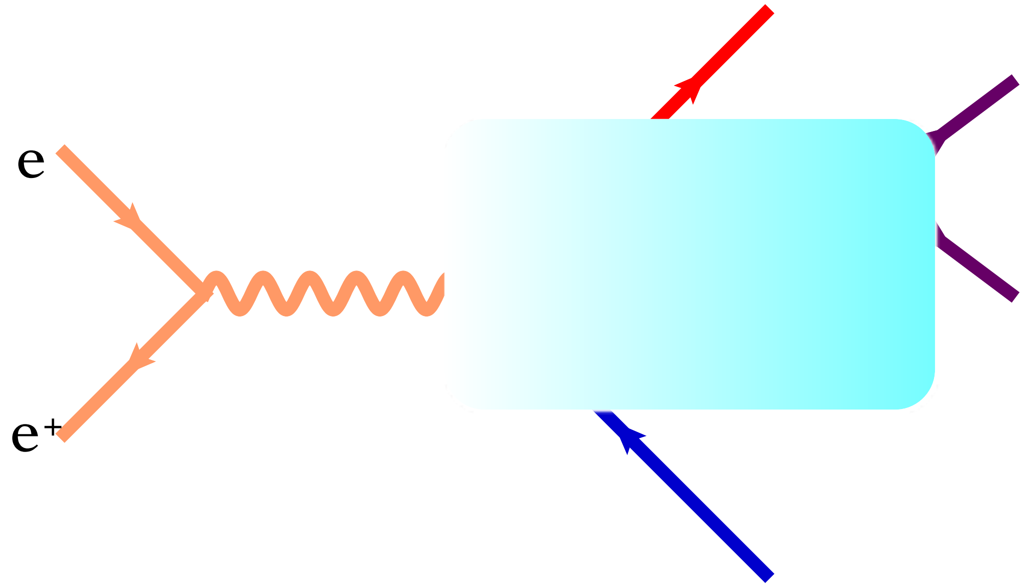
Leading Logarithmic approximation of the matrix element BUT with α_s evaluated at the scale of each splitting

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

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

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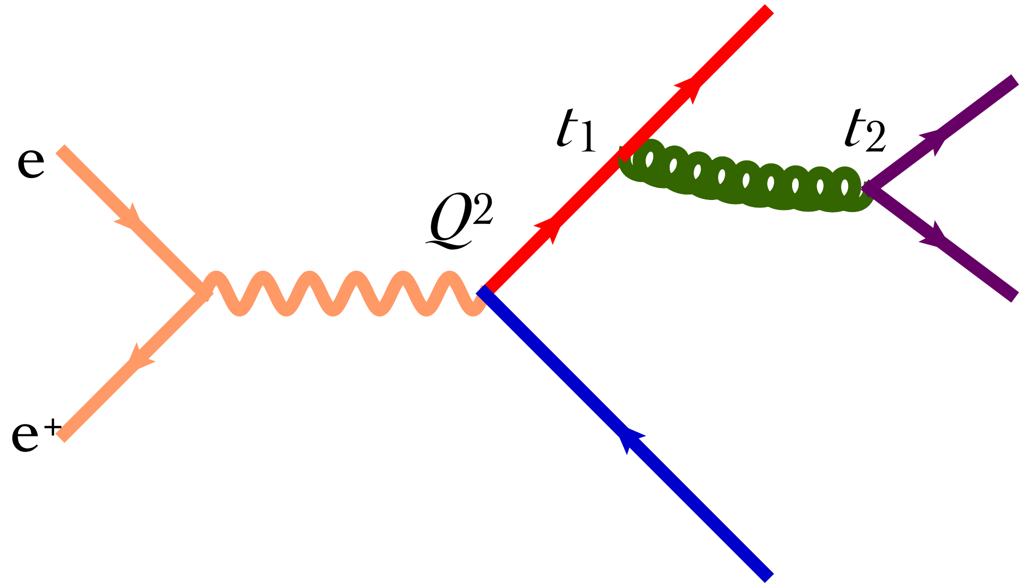

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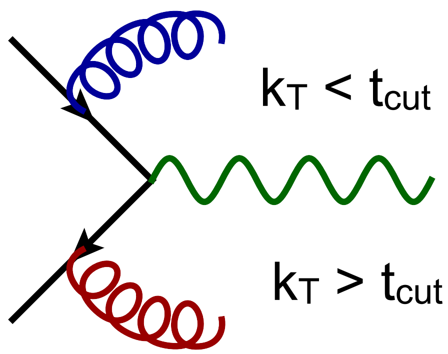
Merging ME with PS

CKKW (2004) and MLM (2004)

- In summary:
- Double counting no problem: we simply throw events away when the matrix-element partons are too soft, or when the parton shower generates too hard radiation
- Applying the matrix-element cut is easy: during phase-space integration, we only generate events with partons above the matching scale

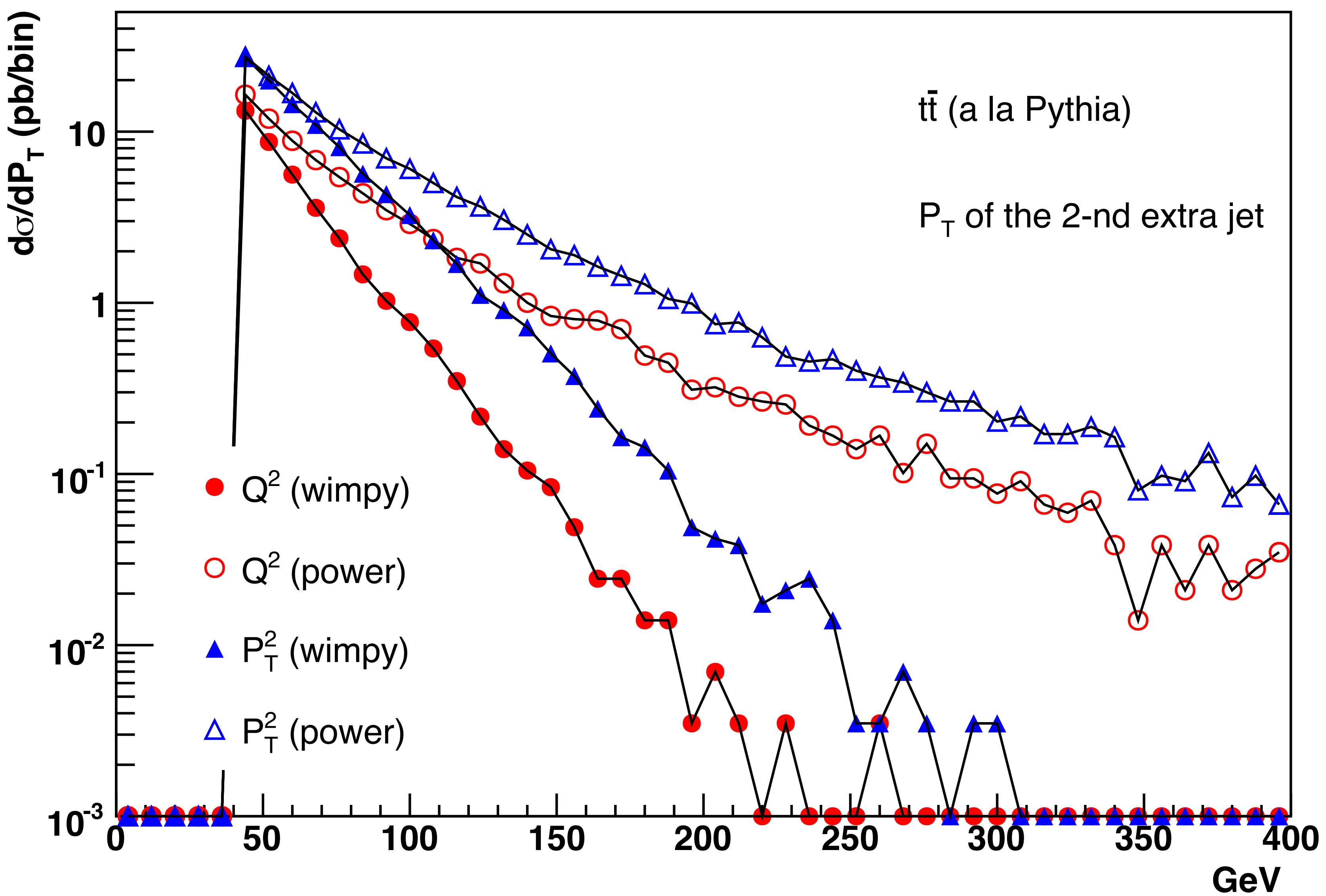


- For the cut on the shower, there are two methods. Throwing events away after showering is not very efficient, although it is working ("MLM method")
- Instead we can also multiply the Born matrix elements by suitable product of Sudakov factors (i.e. the no-emission probabilities) $\Delta(Q_{max}, t_{cut})$ and start the shower at the scale t_{cut} ("CKKW method").
- For a given multiplicity we have

$$\sigma_{n,\mathrm{excl}}^{\mathrm{LO}} = B_n \Theta(k_{T,n} - t_{\mathrm{cut}}) \Delta_n(Q, t_{\mathrm{cut}})$$

Collinear approximation

- Dependence on internal parameters reduced
  - greater predictive power!



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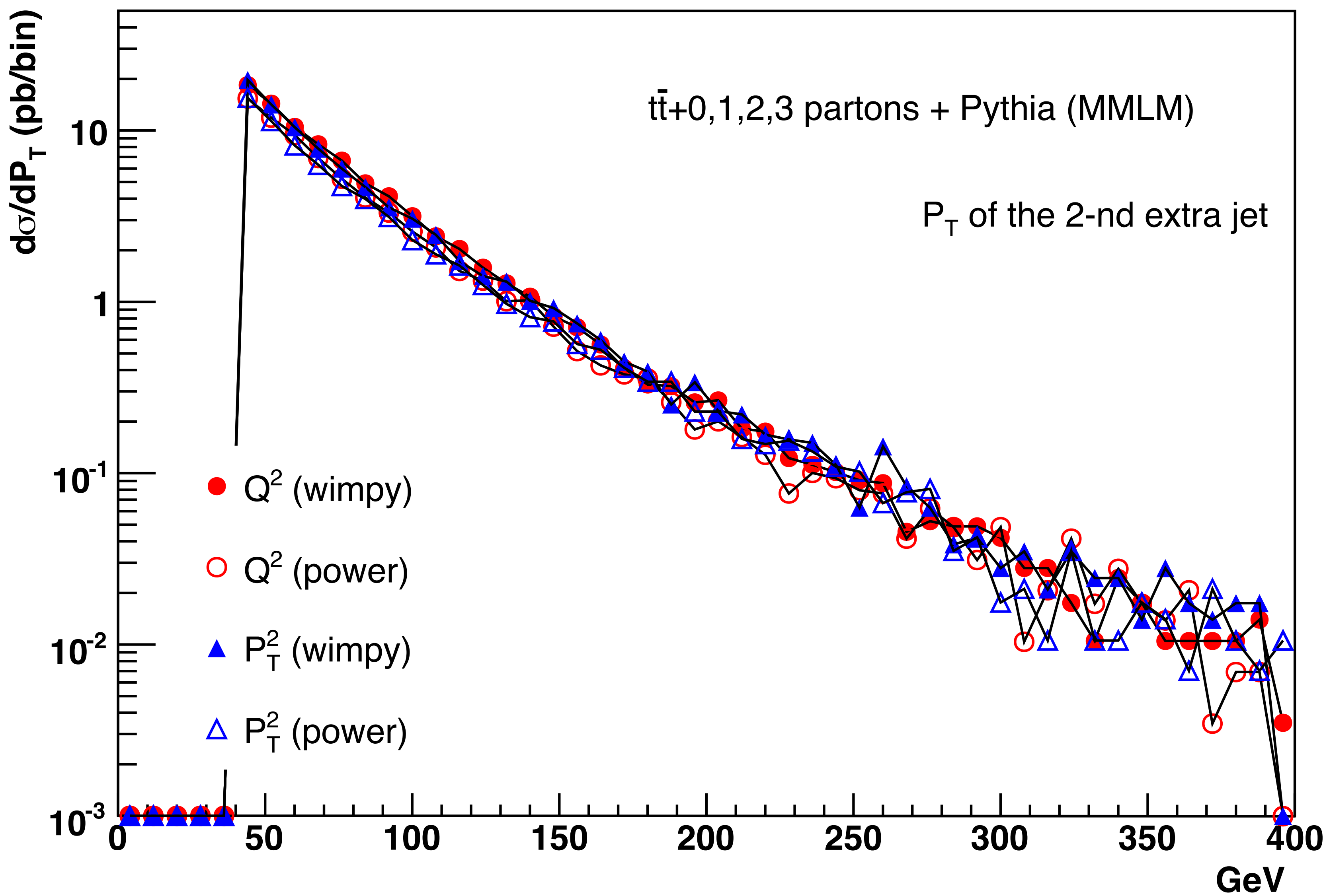
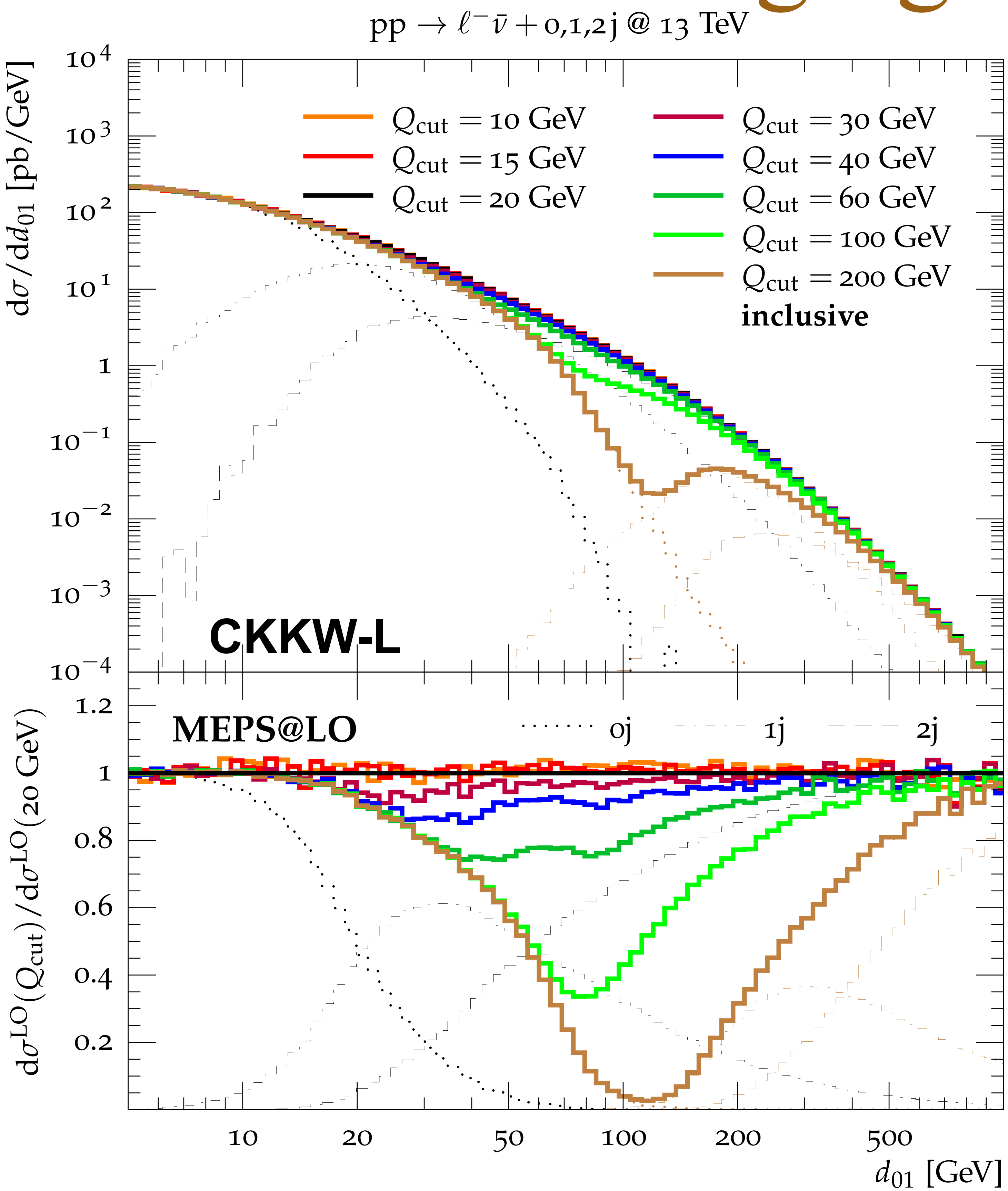


Merging results



- 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

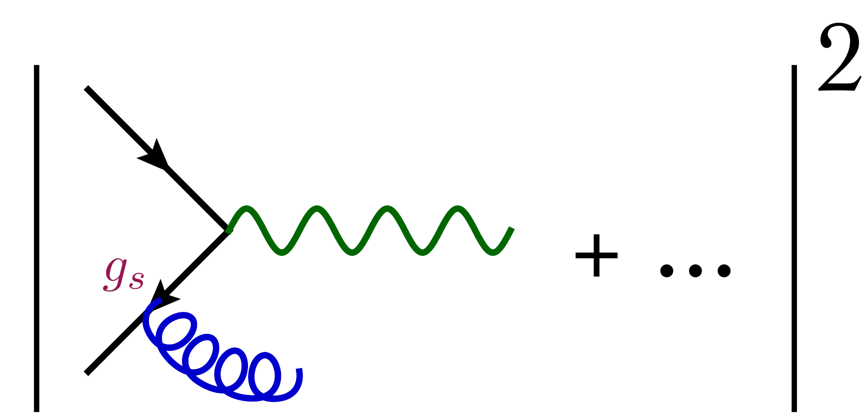
[Kallweit, Lindert, Maierhöfer, Pozzorini, Schönherr 2016]

ME+PS (at LO)

- Merging matrix elements of various multiplicities with parton showers improves the predictive power of the parton shower outside the collinear/soft regions
  - These merged samples give good description of the data (except for the total normalisation)
- There is a dependence on the parameters responsible for the cut in phase-space (i.e. the matching scale)
- By letting the matrix elements mimic what the parton shower does in the collinear/soft regions (PDF/alpha_s reweighting and including the Sudakov suppression) the dependence is greatly reduced
- In practice, one should check explicitly that this is the case by plotting differential jet-rate plots for a couple of values for the matching scale

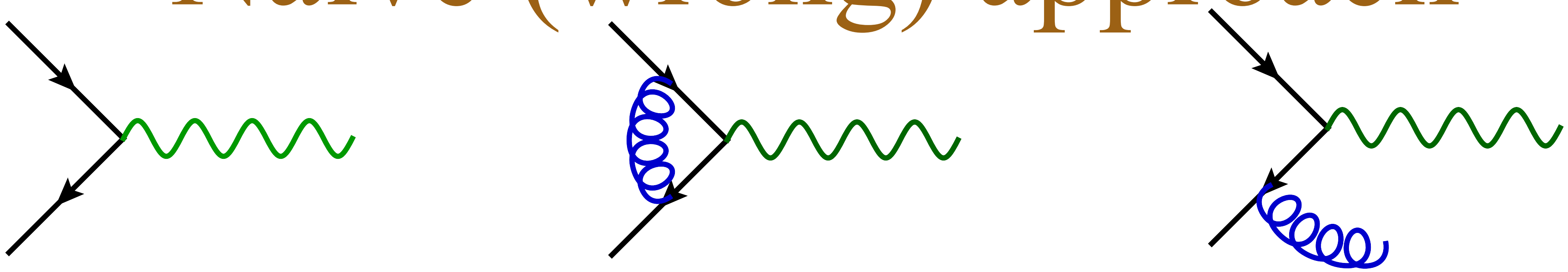
Improving Parton Showers: NLO matching

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

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

- 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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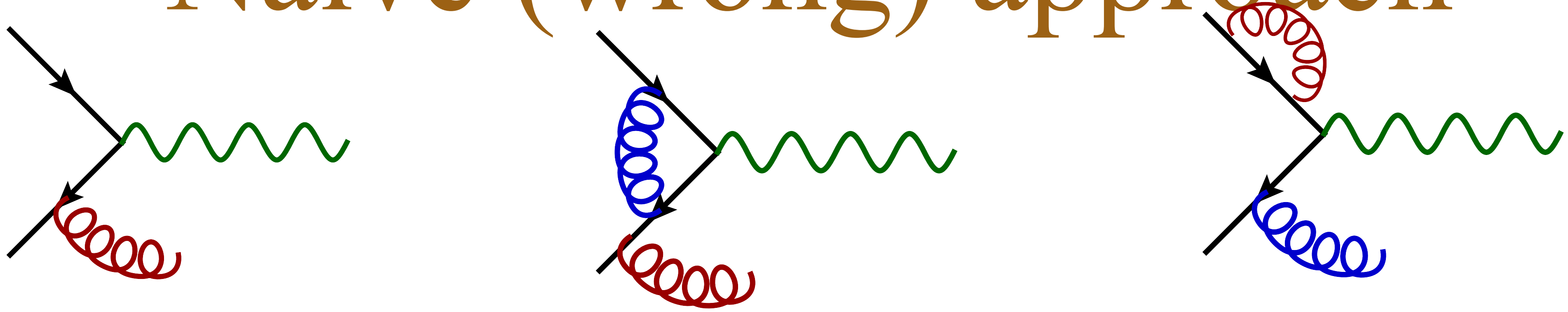

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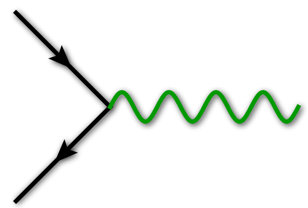
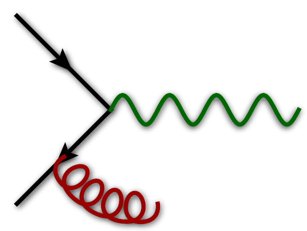
NLO+PS: sources of double counting

Parton shower

Born+Virtual: 

Real emission: 

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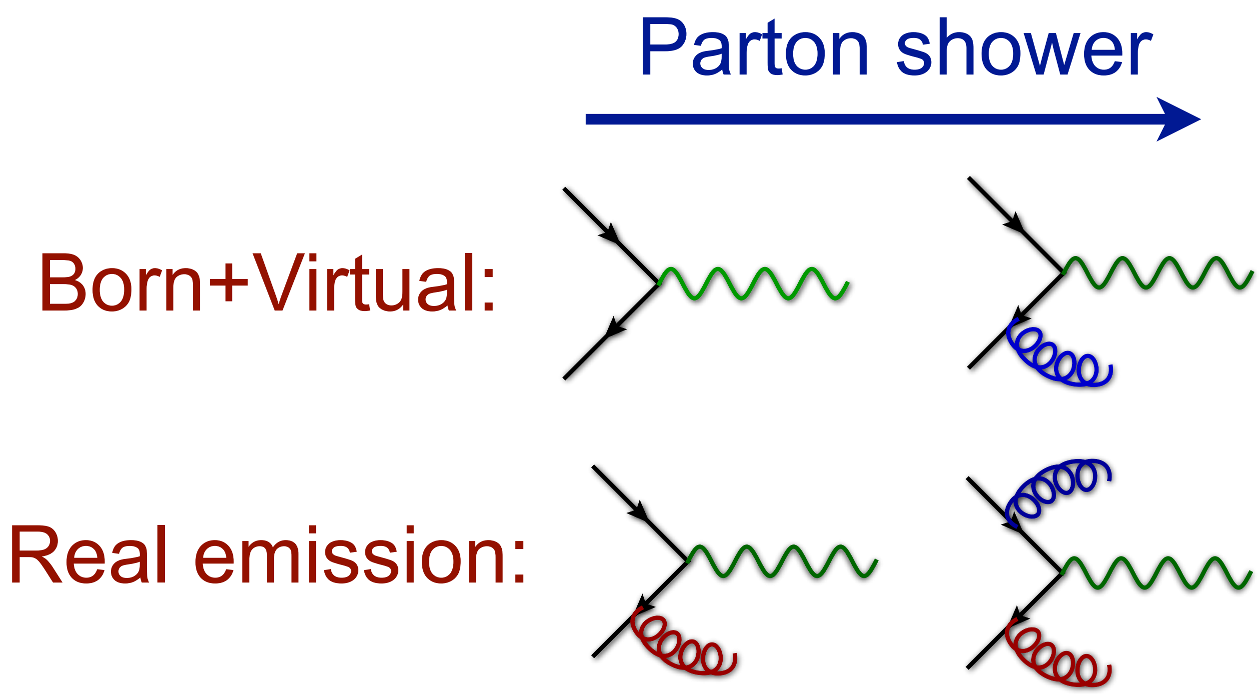

NLO+PS: sources of double counting

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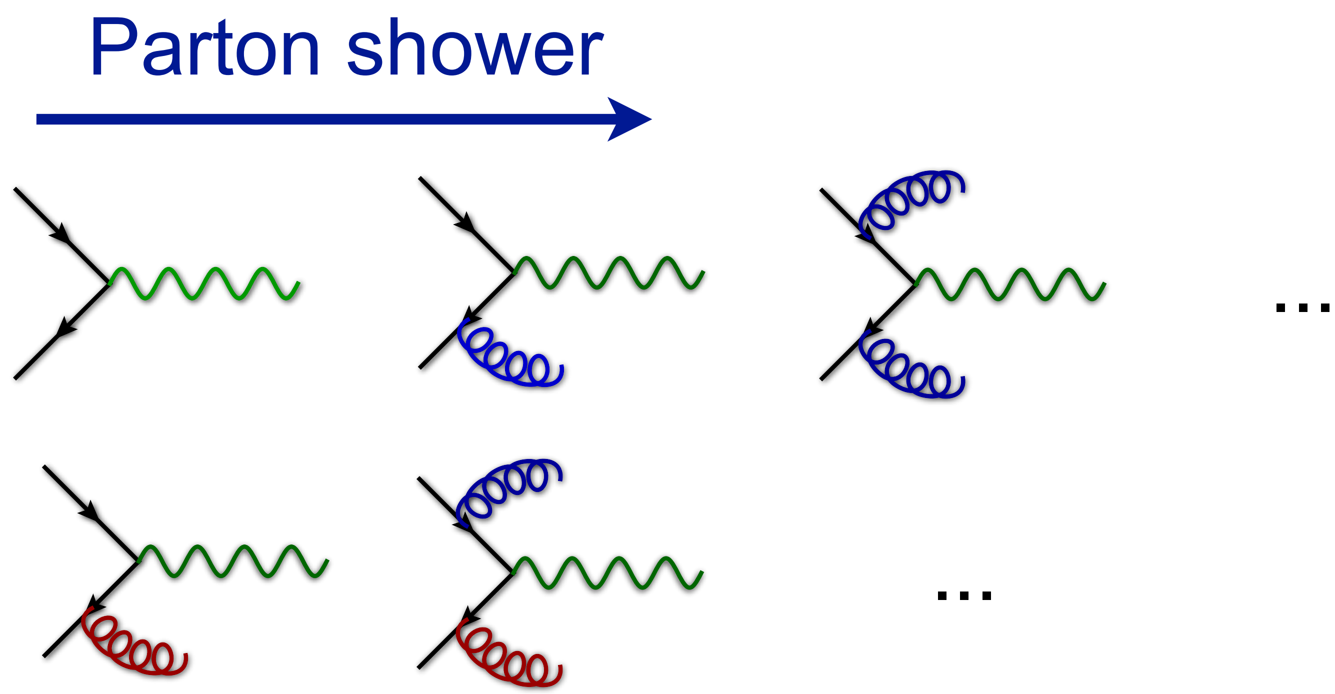

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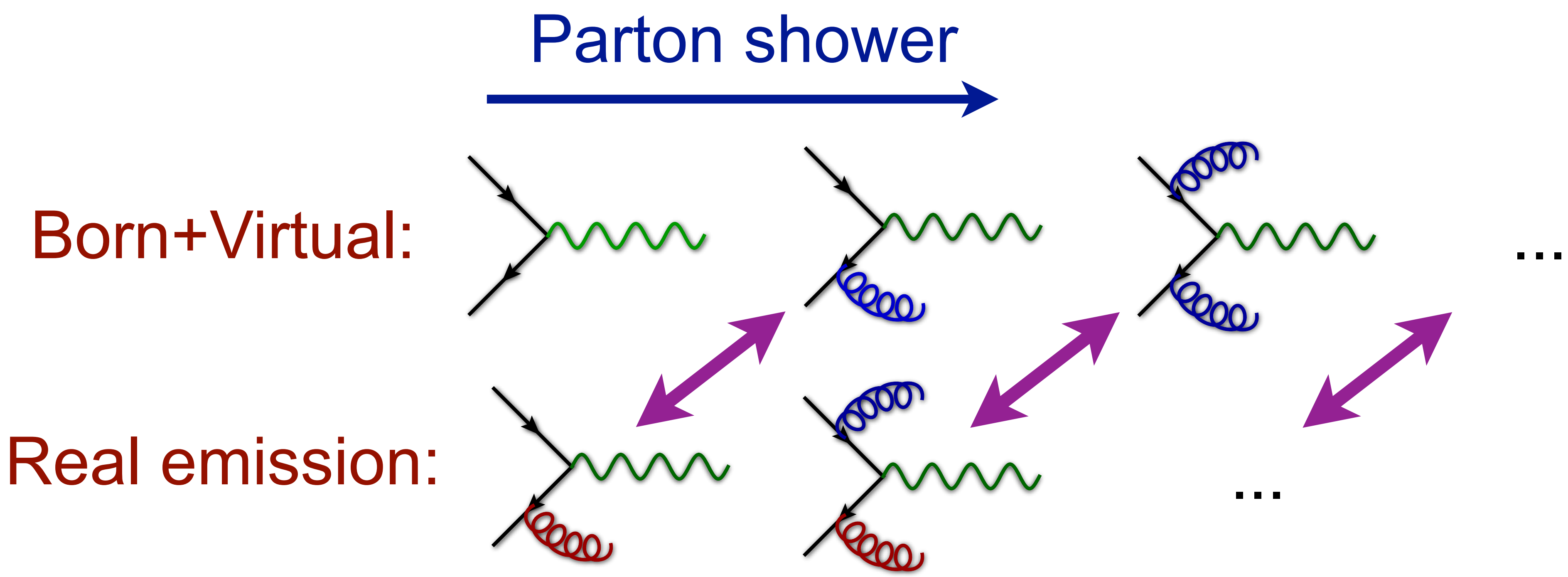

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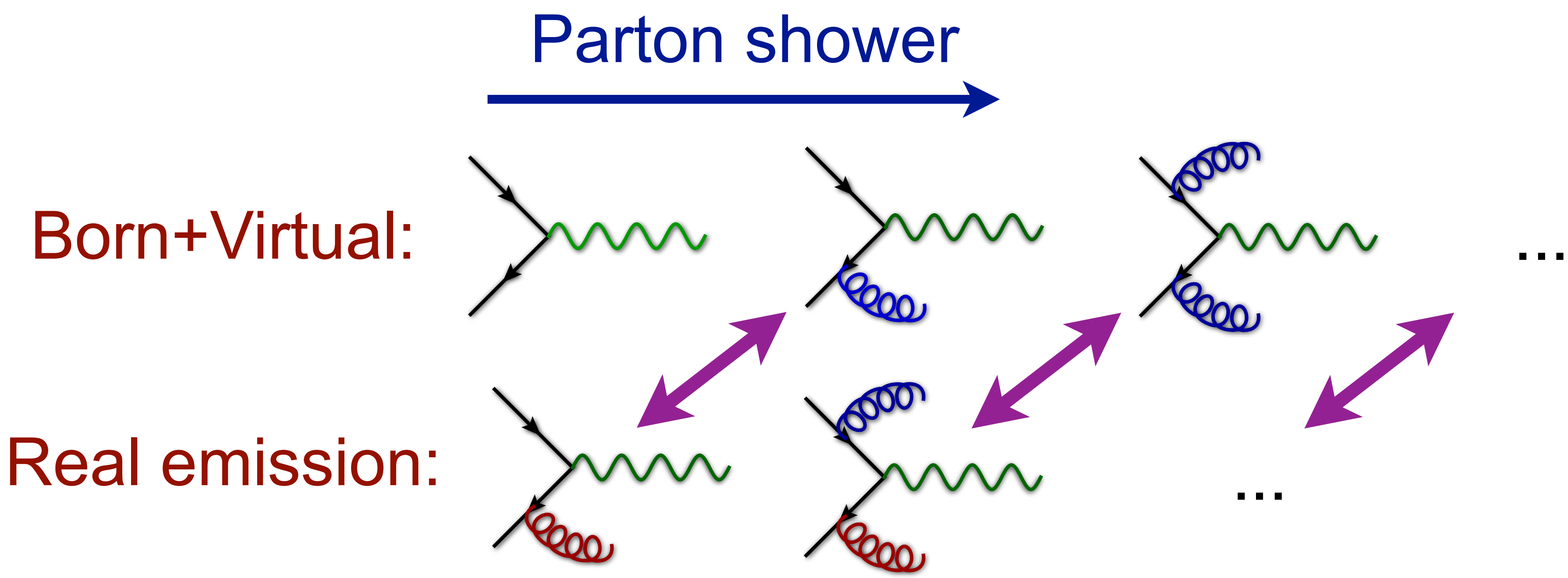


- There is double counting between the real emission matrix elements and the parton shower: the extra radiation can come from the matrix elements or the parton shower
- There is also an overlap between the virtual corrections and the Sudakov suppression in the zero-emission probability
- We have to integrate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

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 two widely methods to circumvent this double counting
  - MC@NLO (Frixione & Webber)
  - POWHEG (Nason)

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

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

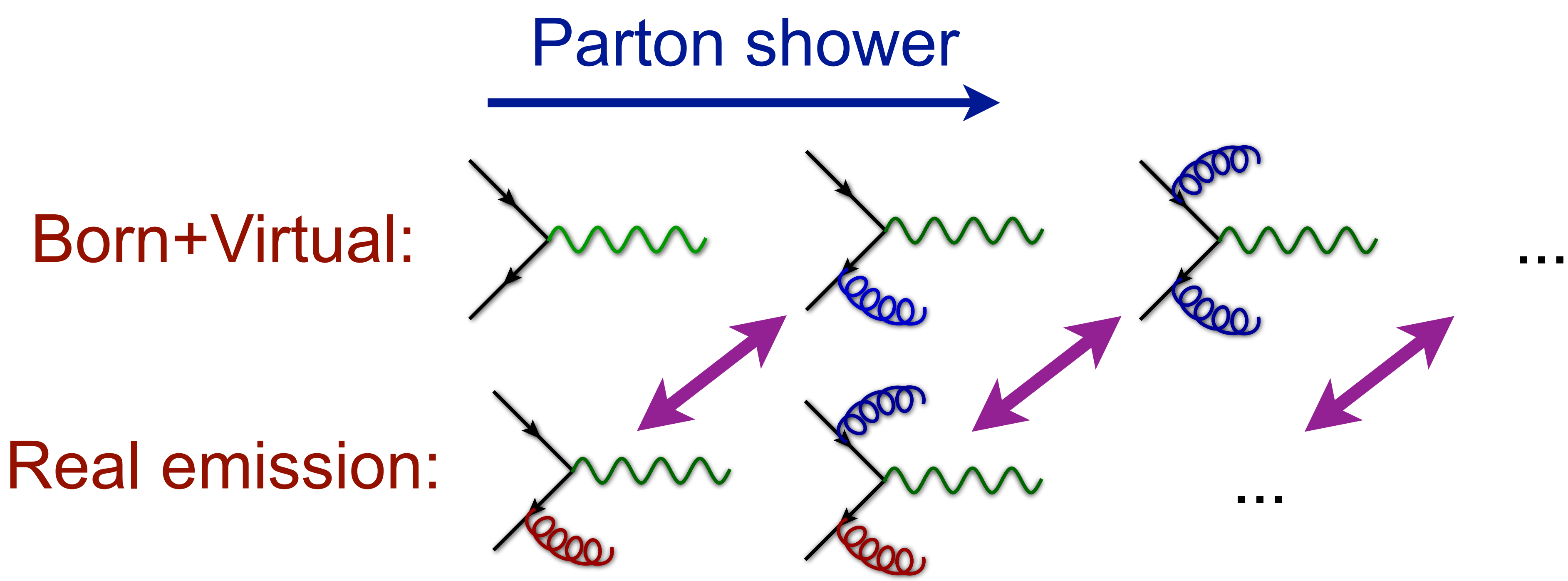
$$+ \left[d\Phi_{m+1} (R - MC) \right]) I_{\mathrm{MC}}^{(m+1)}(O)$$

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

$$MC \equiv B \times \frac{dt}{t} dz \frac{d\phi}{2\pi} \frac{\alpha_s}{2\pi} P_{a\to bc}(z)$$

$$\Delta(Q^2, t) = \exp\left[- \int_t^{Q^2} dp(t') \right] \equiv \exp\left[- \int_t^{Q^2} d\Phi_{+1} \frac{MC}{B} \right]$$

MC@NLO procedure



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

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

$$+ \left[d\Phi_{m+1} (R - MC) \right]) I_{\mathrm{MC}}^{(m+1)}(O)$$

Negative weights

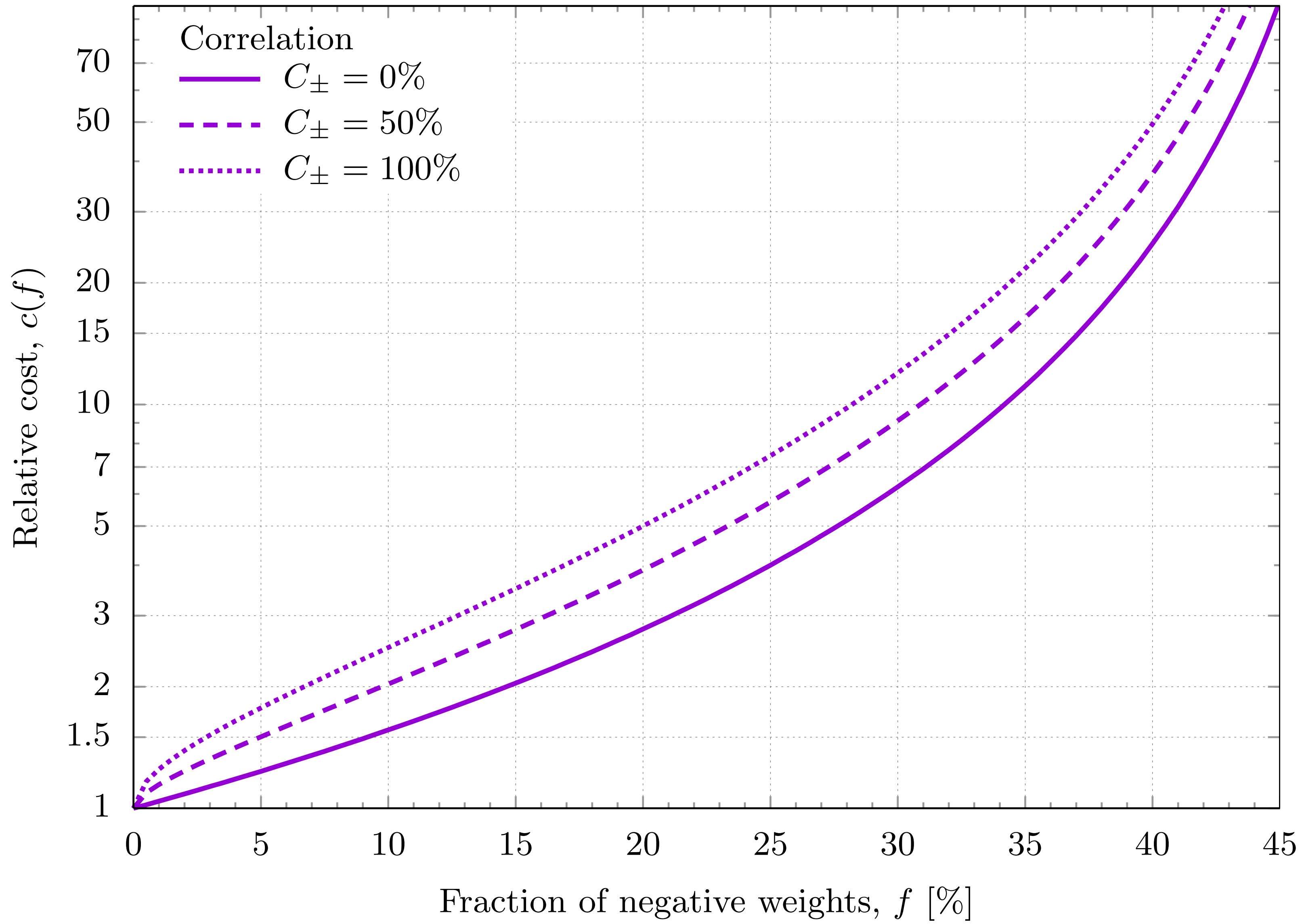
$$\frac{d\sigma_{\mathrm{MC@NLO}}}{dO} = \left[d\Phi_m (B + \int_{\mathrm{loop}} V + \int d\Phi_1 MC) \right] I_{\mathrm{MC}}^{(m)}(O)$$

$$+ \left[d\Phi_{m+1} (R - MC) \right]) I_{\mathrm{MC}}^{(m+1)}(O)$$

- 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

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:



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

$$d\Phi_B \left[B + V + \int d\Phi_{(+1)} R\right] \left[1 - \int d\Phi_{(+1)} \frac{MC}{B} + d\Phi_{(+1)} \frac{MC}{B}\right]$$

  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

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

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Properties

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

- 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 normalization rescaled by a global K-factor and a different Sudakov for the first emission: no negative weights are involved.

NLO+PS

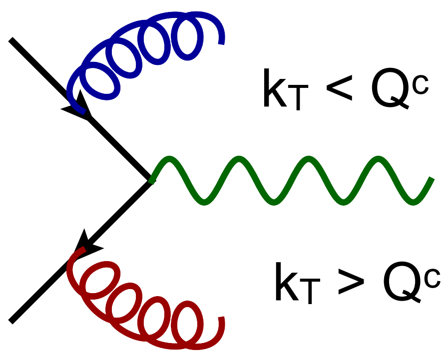
- Advantages:
  - Total cross section and differential distributions related to the hard process are NLO accurate
  - Reduced renormalisation and factorisation scale uncertainties
  - Shower to include multiple emissions; there are models for hadronisation and underlying event
    - Fully exclusive description of the event
- Disadvantages
  - Other observables (e.g., "multi-jet") are only LO accurate, or only generated by the shower

Merging ME+PS at NLO accuracy

Merging LO ME with PS

CKKW (2004) and MLM (2004)

- In summary:
- Double counting no problem: we simply throw events away when the matrix-element partons are too soft, or when the parton shower generates too hard radiation
- Applying the matrix-element cut is easy: during phase-space integration, we only generate events with partons above the matching scale



- For the cut on the shower, there are two methods. Throwing events away after showering is not very efficient, although it is working ("MLM method")
- Instead we can also multiply the Born matrix elements by suitable product of Sudakov factors (i.e. the no-emission probabilities) $\Delta(Q^{max}, Q^c)$ and start the shower at the scale Q^c ("CKKW method").
- For a given multiplicity we have

$$\sigma_{n,\text{excl}}^{\text{LO}} = B_n \Theta(k_{T,n} - Q^c) \Delta_n(Q_{\max}, Q^c)$$

Merging at NLO

- To make a LO prediction exclusive in the number of jets, we need to multiply it by a Sudakov damping factor; this is CKKW method:

$$\sigma^{\mathrm{LO}}_{n,\mathrm{excl}} = B_n \Theta(k_{T,n} - Q^c)\Delta_n(Q_{\mathrm{max}}, Q^c)$$

  This makes the prediction exclusive at leading logarithmic accuracy

- Similarly we can make an NLO prediction exclusive at leading logarithm

$$\sigma^{\mathrm{NLO}}_{n,\mathrm{excl,\ LL}} = \left\{ B_n + V_n + \int d\Phi_1\, R_{n+1} \right\} \Theta(k_{T,n} - Q^c)\Delta_n(Q_{\mathrm{max}}, Q^c)$$

- We can improve here and use the real-emission matrix elements instead of just the Sudakov:

$$\sigma^{\mathrm{NLO}}_{n,\mathrm{excl,\ LL}} = \left\{ B_n + V_n + \int_0^{Q^c} d\Phi_1\, R_{n+1} - B_n \Delta^{(1)}_n(Q_{\mathrm{max}}, Q^c) \right\}$$
$$\Theta(k_{T,n} - Q^c)\Delta_n(Q_{\mathrm{max}}, Q^c)$$

Exclusive MC@NLO: FxFx merging and MEPS@NLO

- Converting the NLO exclusive predictions in the number of jets to the MC@NLO event generation is straight-forward:

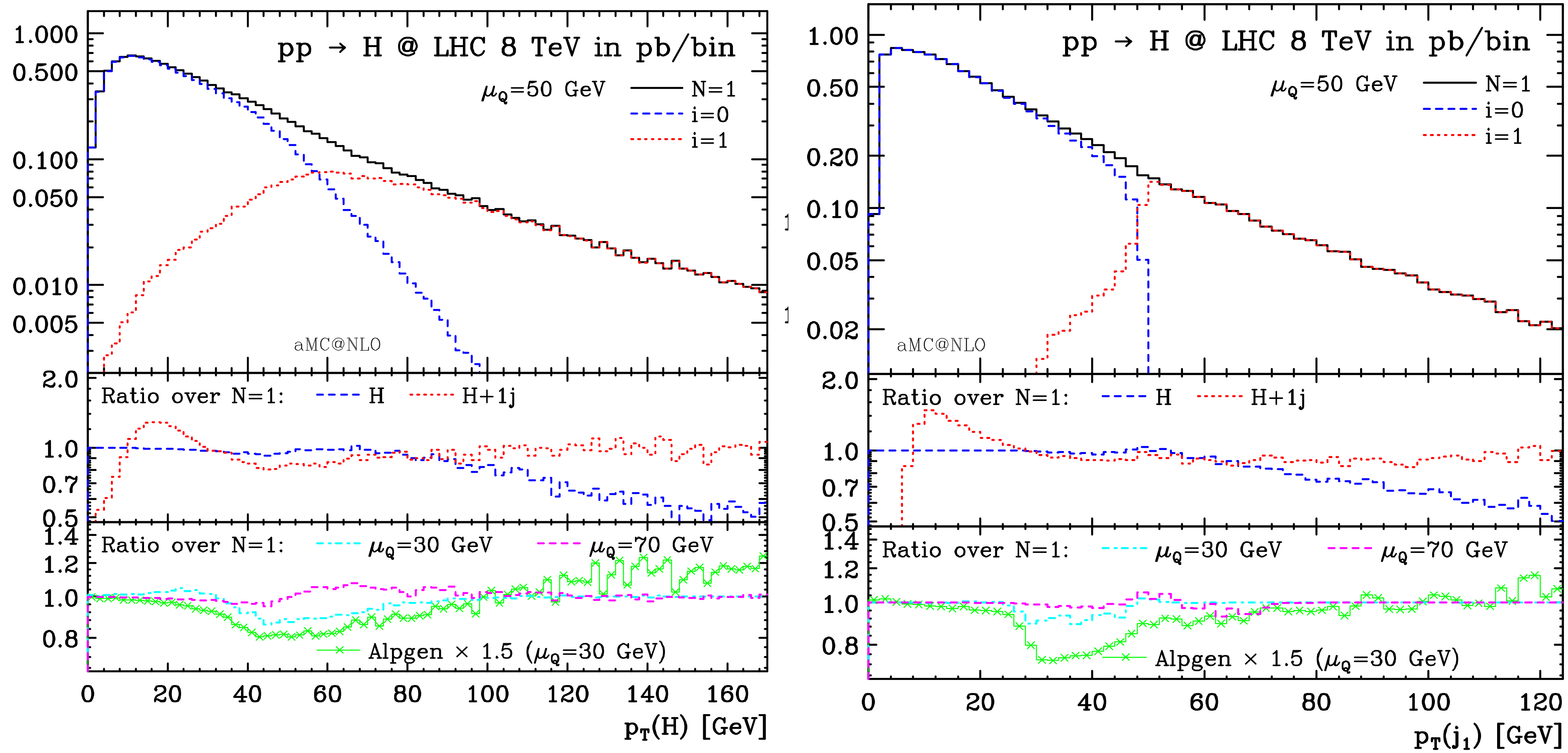
$$\mathbb{S}\text{-events:} \quad \left\{ B_n + V_n + \int_0^{Q^c} d\Phi_1 \, \mathrm{MC} - B_n \Delta_n^{(1)}(Q_{\max}, Q^c) \right\} \Theta(k_{T,n}^B - Q^c) \Delta_n(Q_{\max}^B, Q^c)$$

$$\mathbb{H}\text{-events:} \quad \left\{ R_{n+1} \Theta(k_{T,n}^R - Q^c) - \mathrm{MC} \, \Theta(k_{T,n}^B - Q^c) \right\} \Theta(Q^c - k_{T,n+1}^R) \Delta_n(Q_{\max}^R, Q^c)$$

- But the evil is in the details…

FxFx merging: Higgs boson production

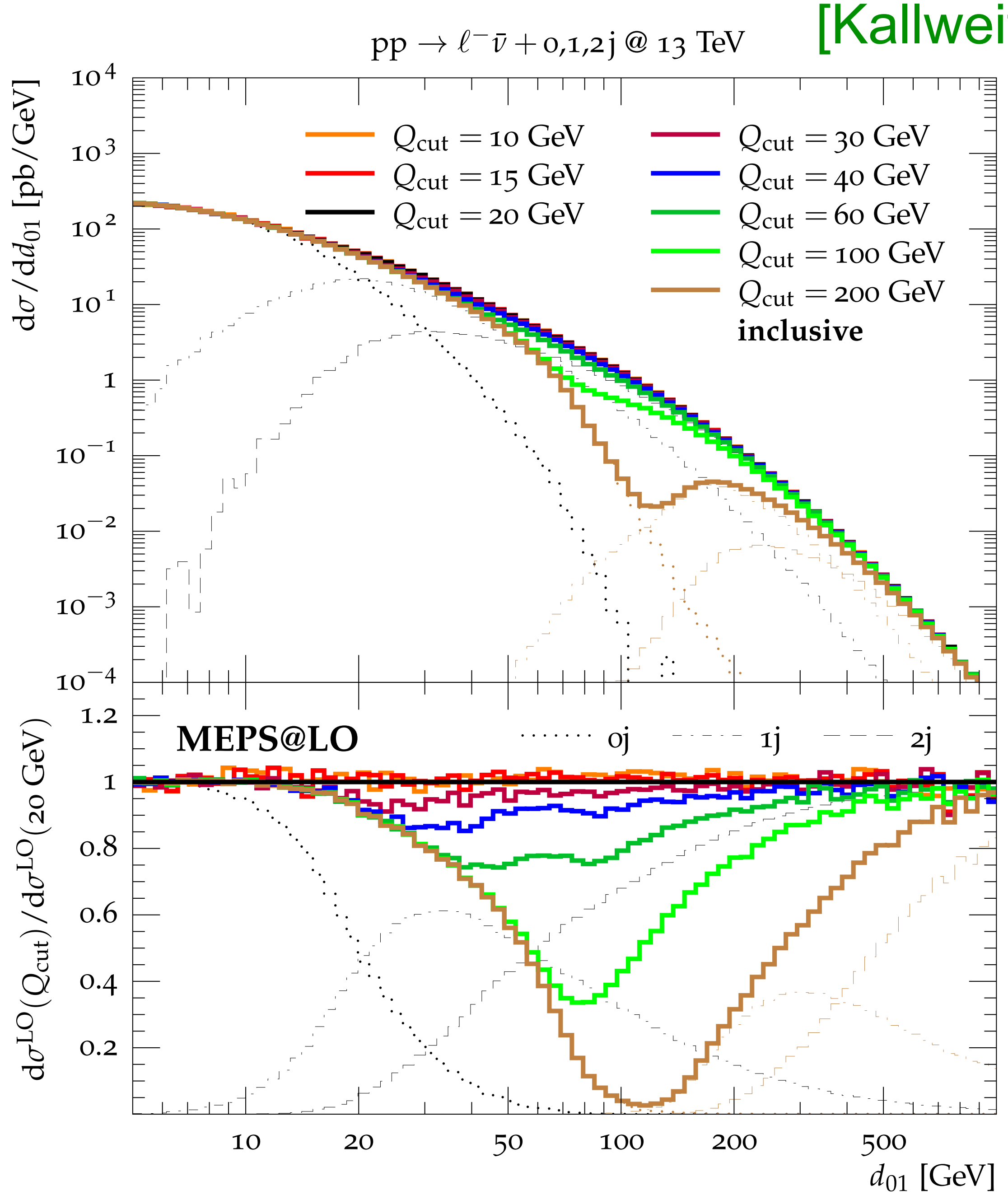
[RF and Frixione]

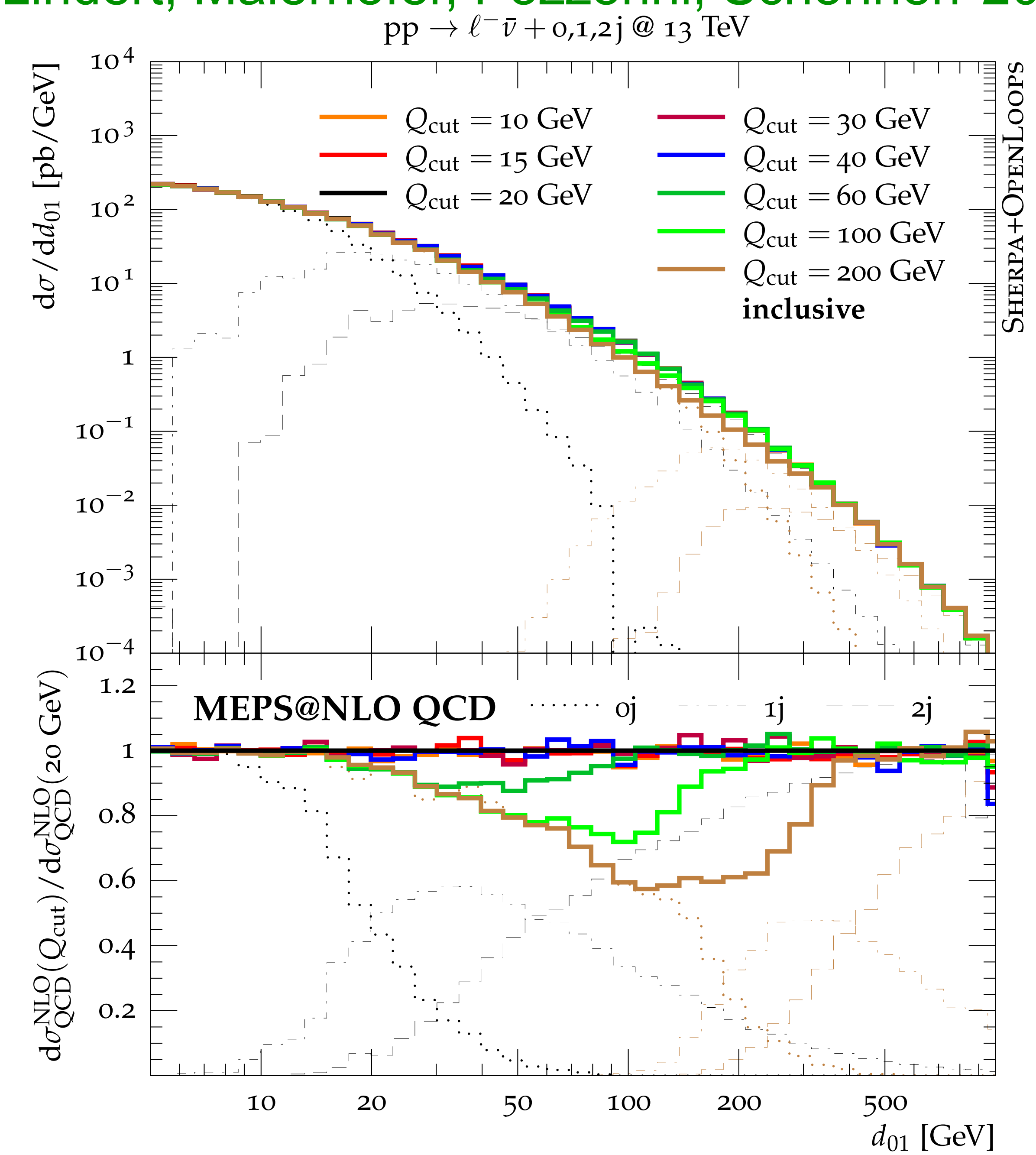


- Transverse momentum of the Higgs and of the 1st jet.
- Agreement with H+0j at MC@NLO and H+1j at MC@NLO in their respective regions of phase-space; Smooth matching in between; Small dependence on matching scale

Merging scale dependence

[Kallweit, Lindert, Maierhöfer, Pozzorini, Schönherr 2016]

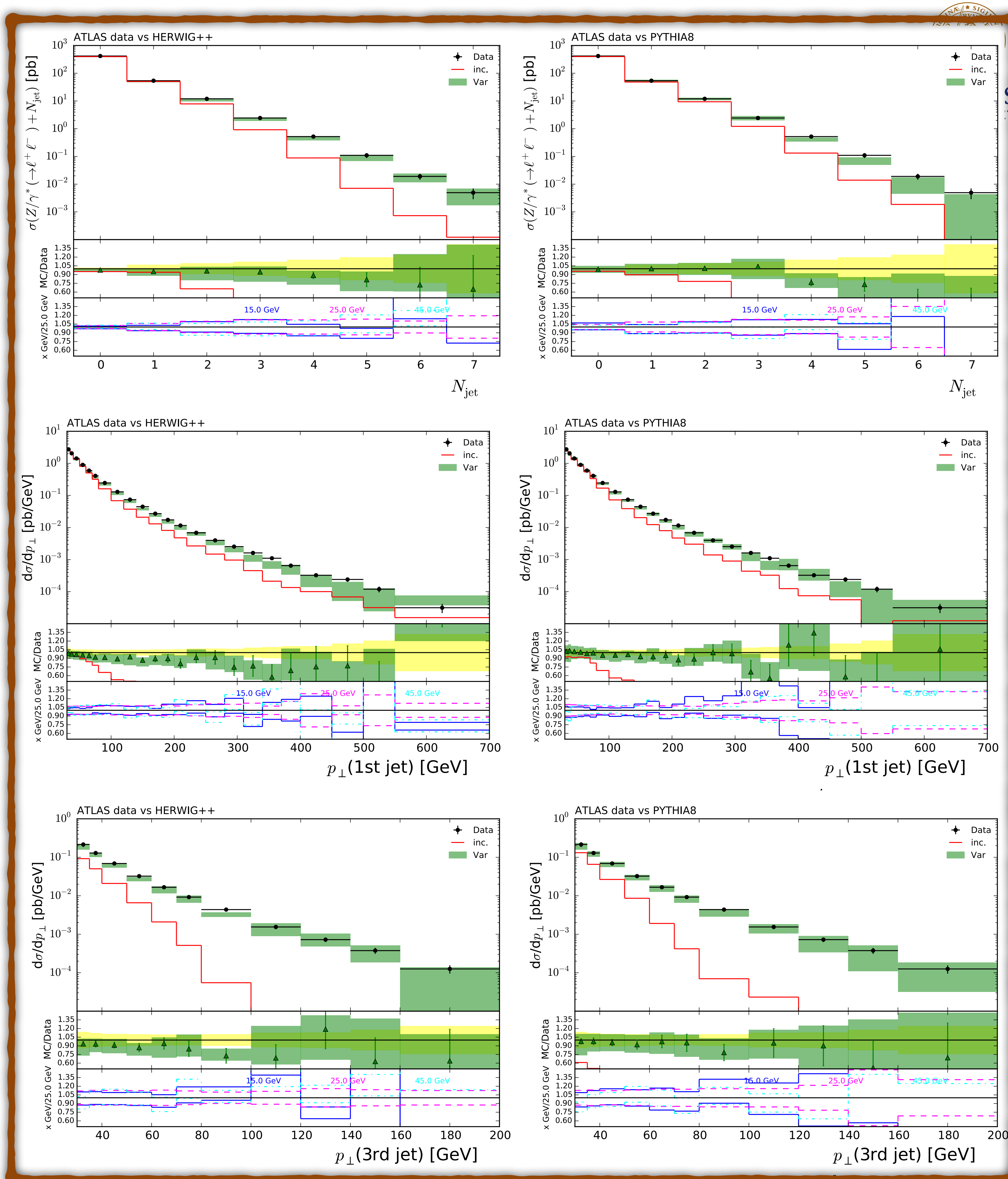




- Besides having the benefits from higher-accurate matrix elements, there is also a **smaller merging scale dependence at NLO**

FxFx

- Comparison to data
- Z+jets
- Exclusive jet multiplicity and hardest and 3rd hardest jet pT spectra
- Uncertainty band contains ren. & fac. scale, PDF & merging scale dependence
- Rather good agreement between data and theory



Conclusions

- In the last couple of years the accuracy of event generation has greatly improved, and full automation has been achieved at NLO accuracy
- A lot of freedom in tuning has been replaced by accurate theory descriptions:
  - More predictive power
  - Better control on uncertainties
  - Greater trust in the measurements
- Recent developments for which I have had no time
  - NLO EW corrections and the parton shower
  - Combining NNLO in QCD and the parton shower: MINNLO
  - MC@NLO-Delta: reducing negative weights in MC@NLO