

QCD and Monte Carlo Methods
Lecture IV: Beyond the tree approximation

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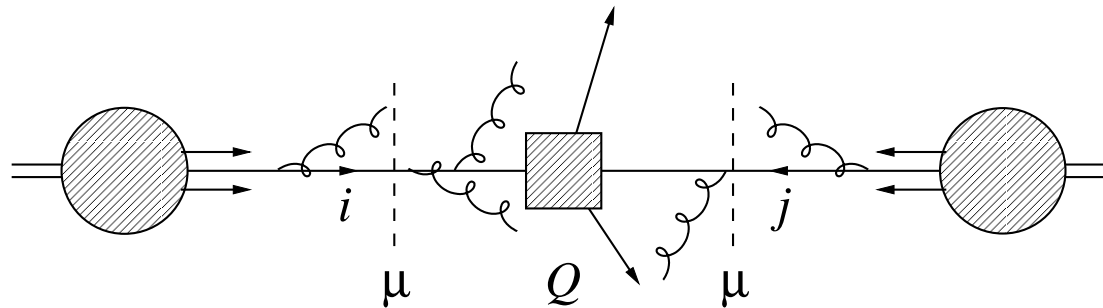
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Beyond the tree approximation

- Hadron-hadron processes and factorization
- W production
 - ★ DY cross section
 - ★ Subtraction method
- Top quark production
- NLO parton integrators
 - ★ Example: MCFM
 - ★ W + jet production
- Combining NLO results with parton showers

Hadron-hadron processes

- In hard hadron-hadron scattering, constituent partons from each incoming hadron interact at short distance (large momentum transfer Q^2).



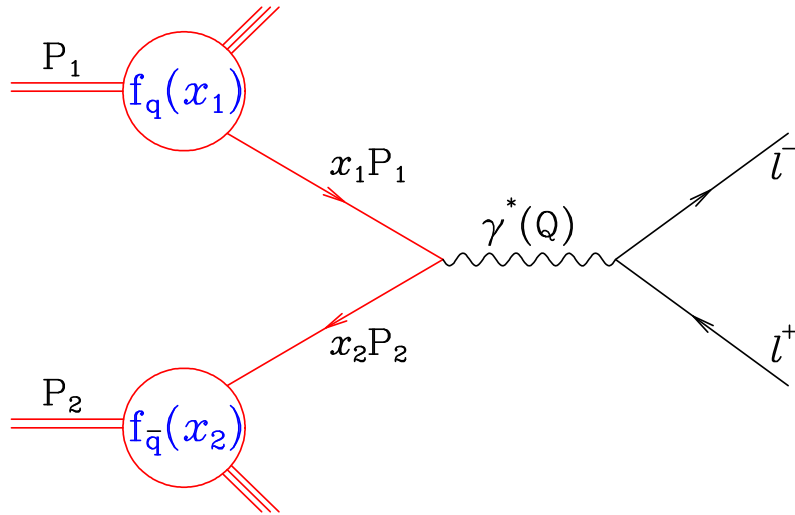
- For hadron momenta P_1, P_2 ($S = 2P_1 \cdot P_2$), form of cross section is

$$\sigma(S) = \sum_{i,j} \int dx_1 dx_2 D_i(x_1, \mu^2) D_j(x_2, \mu^2) \hat{\sigma}_{ij}(\hat{s} = x_1 x_2 S, \alpha_S(\mu^2), Q^2 / \mu^2)$$

where μ^2 is factorization scale and $\hat{\sigma}_{ij}$ is subprocess cross section for parton types i, j .

- ★ Notice that factorization scale is in principle arbitrary: affects only what we call part of subprocess or part of initial-state evolution (parton shower).
- ★ Unlike e^+e^- or ep , we may have interaction between spectator partons, leading to soft underlying event and/or multiple hard scattering.

Lepton-pair production



- Mechanism for Lepton pair production, W -production, Z -production, Vector-boson pairs, ...
- Collectively known as the Drell-Yan process.
- Colour average $1/N$.

$$\frac{d\hat{\sigma}}{dQ^2} = \frac{\sigma_0}{N} Q_q^2 \delta(\hat{s} - Q^2), \quad \sigma_0 = \frac{4\pi\alpha^2}{3Q^2}, \quad \text{cf } e^+e^- \text{ annihilation.}$$

In the CM frame of the two hadrons, the momenta of the incoming partons are

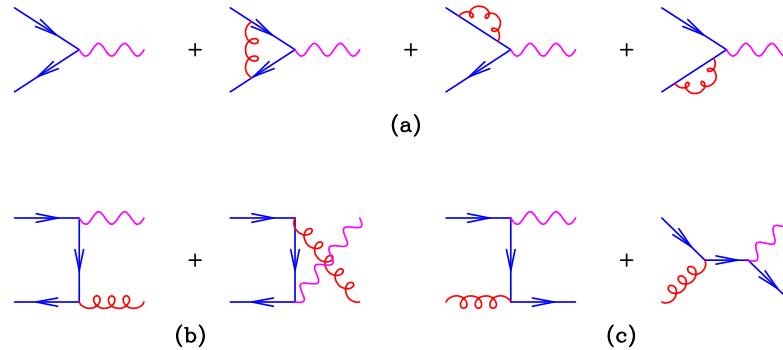
$$p_1 = \frac{\sqrt{s}}{2}(x_1, 0, 0, x_1), \quad p_2 = \frac{\sqrt{s}}{2}(x_2, 0, 0, -x_2).$$

The square of the $q\bar{q}$ collision energy \hat{s} is related to the overall hadron-hadron collision energy by $\hat{s} = (p_1 + p_2)^2 = x_1 x_2 s$. The parton-model cross section for this process is:

$$\begin{aligned} \frac{d\sigma}{dM^2} &= \int_0^1 dx_1 dx_2 \sum_q \{f_q(x_1) f_{\bar{q}}(x_2) + (q \leftrightarrow \bar{q})\} \frac{d\hat{\sigma}}{dM^2}(q\bar{q} \rightarrow l^+ l^-) \\ &= \frac{\sigma_0}{Ns} \int_0^1 \frac{dx_1}{x_1} \frac{dx_2}{x_2} \delta(1-z) \left[\sum_q Q_q^2 \{f_q(x_1) f_{\bar{q}}(x_2) + (q \leftrightarrow \bar{q})\} \right]. \end{aligned}$$

- For later convenience we have introduced the variable $z = \frac{Q^2}{\hat{s}} = \frac{Q^2}{x_1 x_2 s}$.
- The sum here is over quarks only and the $\bar{q}q$ contributions are indicated explicitly.

Next-to-leading order



- The contribution of the real diagrams (in four dimensions) is

$$|M|^2 \sim g^2 C_F \left[\frac{u}{t} + \frac{t}{u} + \frac{2Q^2 s}{ut} \right] = g^2 C_F \left[\left(\frac{1+z^2}{1-z} \right) \left(\frac{-s}{t} + \frac{-s}{u} \right) - 2 \right]$$

where $z = Q^2/s$, $s + t + u = Q^2$.

- Note that the real diagrams contain collinear singularities, $u \rightarrow 0$, $t \rightarrow 0$ and soft singularities, $z \rightarrow 1$.
- The coefficient of the divergence is the unregulated branching probability $\hat{P}_{qq}(z)$.
- Ignore for simplicity the diagrams with incoming gluons.

- Control the divergences by continuing the dimensionality of space-time, $d = 4 - 2\epsilon$, (technically this is dimensional reduction). Performing the phase space integration, the total contribution of the real diagrams is

$$\begin{aligned} \sigma_R = & \frac{\alpha_S}{2\pi} C_F \left(\frac{\mu^2}{Q^2} \right)^\epsilon c_\Gamma \left[\left(\frac{2}{\epsilon^2} + \frac{3}{\epsilon} - \frac{\pi^2}{3} \right) \delta(1-z) - \frac{2}{\epsilon} P_{qq}(z) \right. \\ & \left. - 2(1-z) + 4(1+z^2) \left[\frac{\ln(1-z)}{1-z} \right]_+ - 2 \frac{1+z^2}{(1-z)} \ln z \right] \end{aligned}$$

with $c_\Gamma = (4\pi)^\epsilon / \Gamma(1-\epsilon)$.

- The contribution of the virtual diagrams is

$$\sigma_V = \delta(1-z) \left[1 + \frac{\alpha_S}{2\pi} C_F \left(\frac{\mu^2}{Q^2} \right)^\epsilon c'_\Gamma \left(-\frac{2}{\epsilon^2} - \frac{3}{\epsilon} - 6 + \pi^2 \right) \right]$$

$$c'_\Gamma = c_\Gamma + O(\epsilon^3)$$

- Adding it up we get in dim-reduction

$$\begin{aligned} \sigma_{R+V} &= \frac{\alpha_S}{2\pi} C_F \left(\frac{\mu^2}{Q^2} \right)^\epsilon c_\Gamma \left[\left(\frac{2\pi^2}{3} - 6 \right) \delta(1-z) - \frac{2}{\epsilon} P_{qq}(z) - 2(1-z) \right. \\ &\quad \left. + 4(1+z^2) \left[\frac{\ln(1-z)}{1-z} \right]_+ - 2 \frac{1+z^2}{(1-z)} \ln z \right] \end{aligned}$$

- The divergences, proportional to the branching probability, are universal.
- We will factorize them into the parton distributions. We perform the mass factorization by subtracting the counterterm

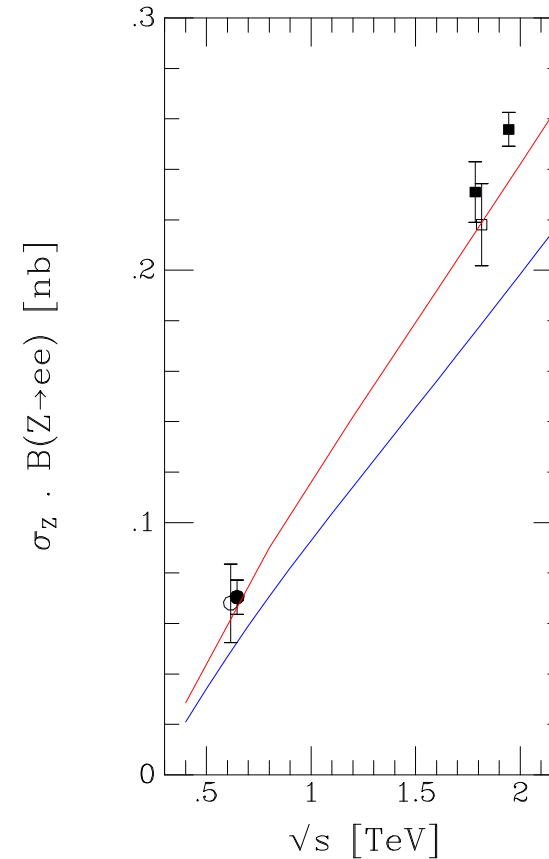
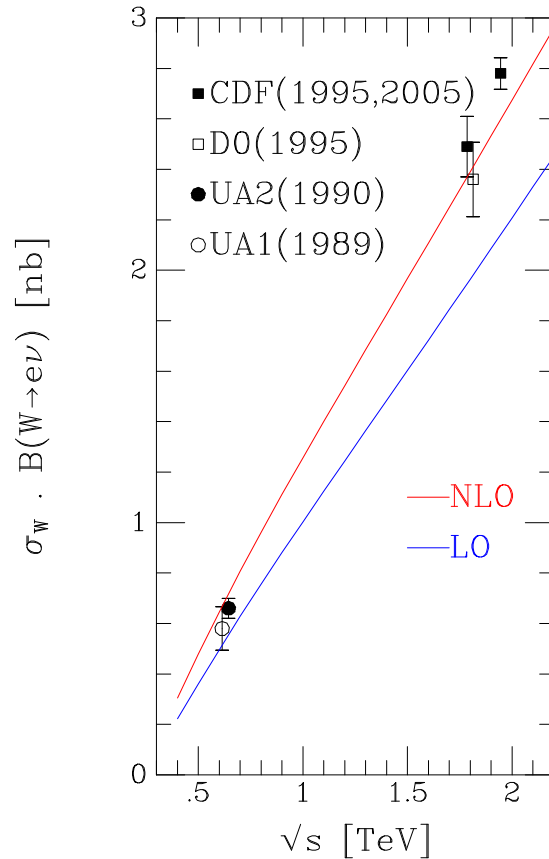
$$2 \frac{\alpha_S}{2\pi} C_F \left[\frac{-c_\Gamma}{\epsilon} P_{qq}(z) - (1-z) + \delta(1-z) \right]$$

(The finite terms are necessary to get us to the \overline{MS} -scheme).

$$\hat{\sigma} = \frac{\alpha_S}{2\pi} C_F \left[\left(\frac{2\pi^2}{3} - 8 \right) \delta(1-z) + 4(1+z^2) \left[\frac{\ln(1-z)}{1-z} \right]_+ - 2 \frac{1+z^2}{(1-z)} \ln z + 2 P_{qq}(z) \ln \frac{Q^2}{\mu^2} \right]$$

- Similar correction for incoming gluons.

Application to W, Z production



- Agreement with NLO theory is good.
- LO curves lie about 25% too low.
- NNLO results are also known and lead to a further modest (4%) increase at the Tevatron.

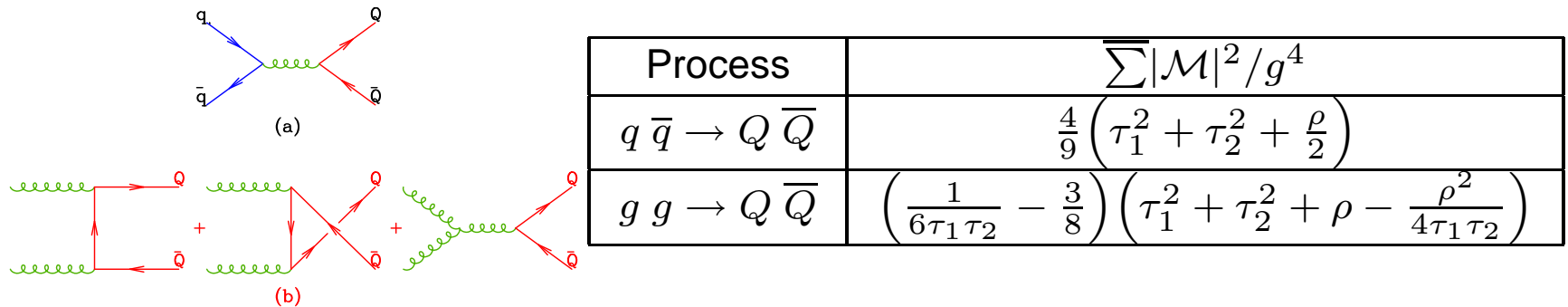
Heavy quark production, leading order

The leading-order processes for the production of a heavy quark Q of mass m in hadron-hadron collisions

$$(a) \quad q(p_1) + \bar{q}(p_2) \rightarrow Q(p_3) + \bar{Q}(p_4)$$

$$(b) \quad g(p_1) + g(p_2) \rightarrow Q(p_3) + \bar{Q}(p_4)$$

where the four-momenta of the partons are given in brackets.



$\overline{\sum}$ indicates averaged (summed) over initial (final) colours and spins. We have introduced the following notation for the ratios of scalar products:

$$\tau_1 = \frac{2p_1 \cdot p_3}{\hat{s}}, \quad \tau_2 = \frac{2p_2 \cdot p_3}{\hat{s}}, \quad \rho = \frac{4m^2}{\hat{s}}, \quad \hat{s} = (p_1 + p_2)^2.$$

- The short-distance cross section is obtained from the invariant matrix element in the usual way:

$$d\hat{\sigma}_{ij} = \frac{1}{2\hat{s}} \frac{d^3p_3}{(2\pi)^3 2E_3} \frac{d^3p_4}{(2\pi)^3 2E_4} (2\pi)^4 \delta^4(p_1 + p_2 - p_3 - p_4) \overline{\sum} |\mathcal{M}_{ij}|^2.$$

The first factor is the flux factor for massless incoming particles. The other terms come from the phase space for $2 \rightarrow 2$ scattering.

- In terms of the rapidity $y = \frac{1}{2} \ln((E + p_z)/(E - p_z))$ and transverse momentum, p_T , the relativistically invariant phase space volume element of the final-state heavy quarks is

$$\frac{d^3p}{E} = dy d^2p_T .$$

The result for the invariant cross section may be written as

$$\frac{d\sigma}{dy_3 dy_4 d^2 p_T} = \frac{1}{16\pi^2 \hat{s}^2} \sum_{ij} x_1 f_i(x_1, \mu^2) x_2 f_j(x_2, \mu^2) \overline{\sum} |\mathcal{M}_{ij}|^2.$$

x_1 and x_2 are fixed if we know the transverse momenta and rapidity of the outgoing heavy quarks. In the centre-of-mass system of the incoming hadrons we may write

$$\begin{aligned} p_1 &= \frac{1}{2} \sqrt{s} (x_1, 0, 0, x_1) \\ p_2 &= \frac{1}{2} \sqrt{s} (x_2, 0, 0, -x_2) \\ p_3 &= (m_T \cosh y_3, p_T, 0, m_T \sinh y_3) \\ p_4 &= (m_T \cosh y_4, -p_T, 0, m_T \sinh y_4). \end{aligned}$$

Applying energy and momentum conservation, we obtain

$$x_1 = \frac{m_T}{\sqrt{s}} (e^{y_3} + e^{y_4}), x_2 = \frac{m_T}{\sqrt{s}} (e^{-y_3} + e^{-y_4}), \hat{s} = 2m_T^2 (1 + \cosh \Delta y).$$

The quantity $m_T = \sqrt{(m^2 + p_T^2)}$ is the transverse mass of the heavy quarks and $\Delta y = y_3 - y_4$ is the rapidity difference between them.

In these variables the leading order cross section is

$$\frac{d\sigma}{dy_3 dy_4 d^2 p_T} = \frac{1}{64\pi^2 m_T^4 (1 + \cosh(\Delta y))^2} \sum_{ij} x_1 f_i(x_1, \mu^2) x_2 f_j(x_2, \mu^2) \overline{\sum} |\mathcal{M}_{ij}|^2.$$

Expressed in terms of m , m_T and Δy , the matrix elements for the two processes are

$$\overline{\sum} |\mathcal{M}_{q\bar{q}}|^2 = \frac{4g^4}{9} \left(\frac{1}{1 + \cosh(\Delta y)} \right) \left(\cosh(\Delta y) + \frac{m^2}{m_T^2} \right),$$

$$\overline{\sum} |\mathcal{M}_{gg}|^2 = \frac{g^4}{24} \left(\frac{8 \cosh(\Delta y) - 1}{1 + \cosh(\Delta y)} \right) \left(\cosh(\Delta y) + 2 \frac{m^2}{m_T^2} - 2 \frac{m^4}{m_T^4} \right).$$

- As the rapidity separation Δy between the two heavy quarks becomes large

$$\overline{\sum} |\mathcal{M}_{q\bar{q}}|^2 \sim \text{constant}, \quad \overline{\sum} |\mathcal{M}_{gg}|^2 \sim \exp \Delta y.$$

- The cross section is damped at large Δy and heavy quarks produced by $q\bar{q}$ annihilation are more closely correlated in rapidity those produced by gg fusion.

Applicability of perturbation theory?

- Consider the propagators in the diagrams.

$$\begin{aligned}(p_1 + p_2)^2 &= 2p_1 \cdot p_2 = 2m_T^2 (1 + \cosh \Delta y) , \\(p_1 - p_3)^2 - m^2 &= -2p_1 \cdot p_3 = -m_T^2 (1 + e^{-\Delta y}) , \\(p_2 - p_3)^2 - m^2 &= -2p_2 \cdot p_3 = -m_T^2 (1 + e^{\Delta y}) .\end{aligned}$$

Note that the propagators are all off-shell by a quantity of least of order m^2 .

- Thus for a sufficiently heavy quark we expect the methods of perturbation theory to be applicable. It is the mass m (which by supposition is very much larger than the scale of the strong interactions Λ) which provides the large scale in heavy quark production. We expect corrections of order Λ/m
- This does not address the issue of whether the charm or bottom mass is large enough to be adequately described by perturbation theory.

Heavy quark production in $O(\alpha_S^3)$

In NLO heavy quark production m is the heavy quark mass.

$$\sigma(S) = \sum_{i,j} \int dx_1 dx_2 \hat{\sigma}_{ij}(x_1 x_2 S, m^2, \mu^2) F_i(x_1, \mu^2) F_j(x_2, \mu^2)$$

$$\hat{\sigma}_{i,j}(\hat{s}, m^2, \mu^2) = \sigma_0 c_{ij}(\hat{\rho}, \mu^2)$$

where $\hat{\rho} = 4m^2/\hat{s}$, $\bar{\mu}^2 = \mu^2/m^2$, $\sigma_0 = \alpha_S^2(\mu^2)/m^2$ and \hat{s} is the parton total c-of-m energy squared. The coupling satisfies

$$\frac{d\alpha_S}{d \ln \mu^2} = -b_0 \frac{\alpha_S^2}{2\pi} + O(\alpha_S^3), \quad b_0 = \frac{11N - 2n_f}{6}$$

$$c_{ij}\left(\rho, \frac{\mu^2}{m^2}\right) = c_{ij}^{(0)}(\rho) + 4\pi\alpha_S(\mu^2) \left[c_{ij}^{(1)}(\rho) + \bar{c}_{ij}^{(1)}(\rho) \ln\left(\frac{\mu^2}{m^2}\right) \right] + O(\alpha_S^2)$$

The lowest-order functions $c_{ij}^{(0)}$ are obtained by integrating the lowest order matrix elements

$$c_{q\bar{q}}^{(0)}(\rho) = \frac{\pi\beta\rho}{27} \left[(2 + \rho) \right] ,$$

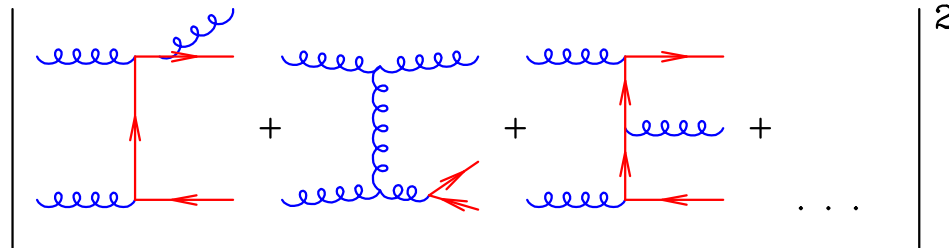
$$c_{gg}^{(0)}(\rho) = \frac{\pi\beta\rho}{192} \left[\frac{1}{\beta} [\rho^2 + 16\rho + 16] \ln \left(\frac{1 + \beta}{1 - \beta} \right) - 28 - 31\rho \right] ,$$

$$c_{gq}^{(0)}(\rho) = c_{g\bar{q}}^{(0)}(\rho) = 0 ,$$

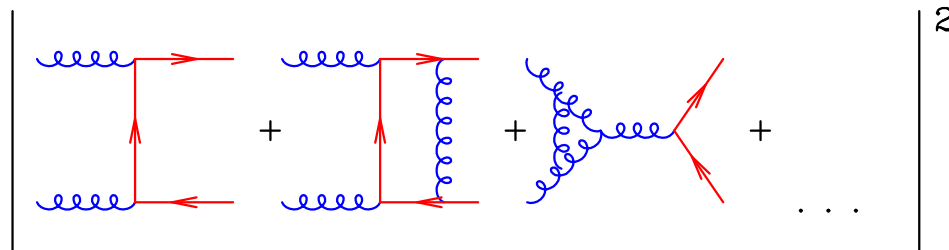
and $\beta = \sqrt{1 - \rho}$.

- The functions $c_{ij}^{(0)}$ vanish both at threshold ($\beta \rightarrow 0$) and at high energy ($\rho \rightarrow 0$).
- Note that the quark-gluon process is zero in lowest order, but is present in higher orders.

- The functions $c_{ij}^{(1)}$ are also known



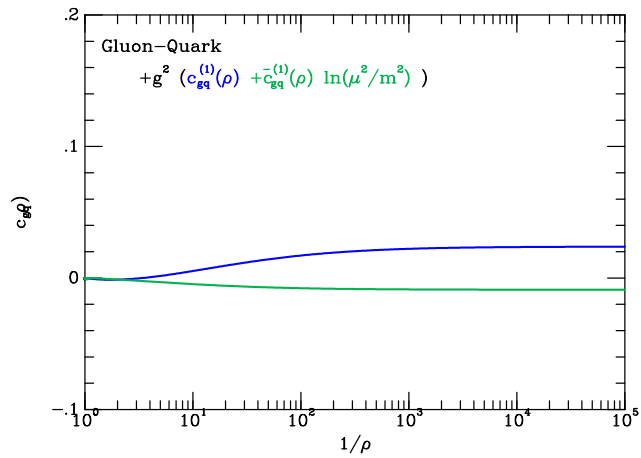
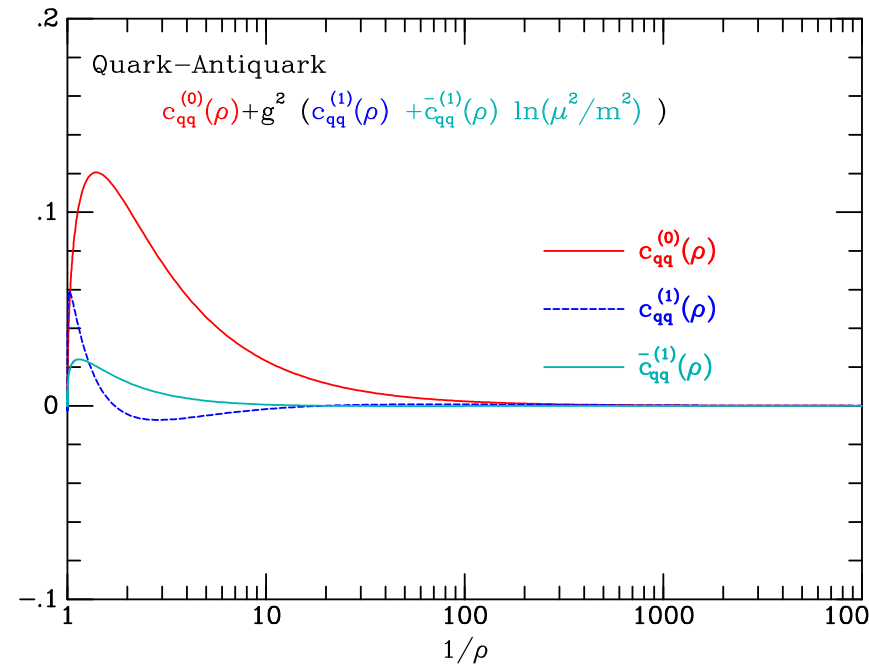
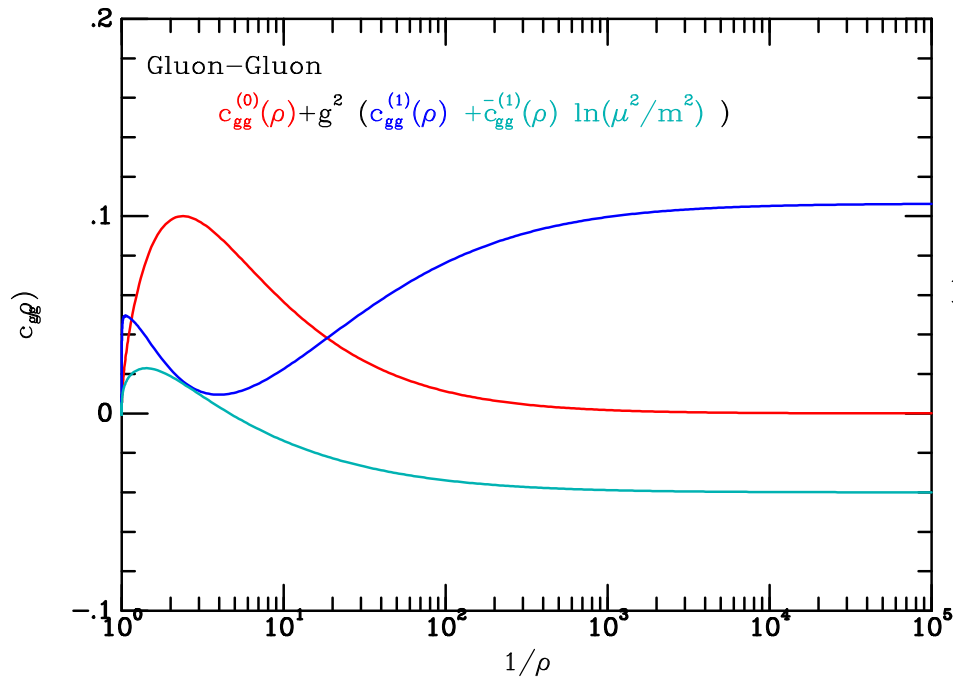
Real emission diagrams



Virtual emission diagrams

- Examples of higher-order corrections to heavy quark production.
- In order to calculate the c_{ij} in perturbation theory we must perform both renormalization and factorization of mass singularities. The subtractions required for renormalization and factorization are done at mass scale μ .

Higher order results, $c_{ij}^{(1)}$



μ dependence

μ is an unphysical parameter. The physical predictions should be invariant under changes of μ at the appropriate order in perturbation theory. If we have performed a calculation to $O(\alpha_S^3)$, variations of the scale μ will lead to corrections of $O(\alpha_S^4)$,

$$\mu^2 \frac{d}{d\mu^2} \sigma = O(\alpha_S^4).$$

- The term $\bar{c}^{(1)}$, which controls the μ dependence of the higher-order perturbative contributions, is fixed in terms of the lower-order result $c^{(0)}$:

$$\begin{aligned} \bar{c}_{ij}^{(1)}(\rho) = & \frac{1}{8\pi^2} \left[4\pi b c_{ij}^{(0)}(\rho) - \int_{\rho}^1 dz_1 \sum_k c_{kj}^{(0)}\left(\frac{\rho}{z_1}\right) P_{ki}^{(0)}(z_1) \right. \\ & \left. - \int_{\rho}^1 dz_2 \sum_k c_{ik}^{(0)}\left(\frac{\rho}{z_2}\right) P_{kj}^{(0)}(z_2) \right]. \end{aligned}$$

In obtaining this result we have used the renormalization group equation for the running coupling

$$\mu^2 \frac{d}{d\mu^2} \alpha_S(\mu^2) = -b\alpha_S^2 + \dots$$

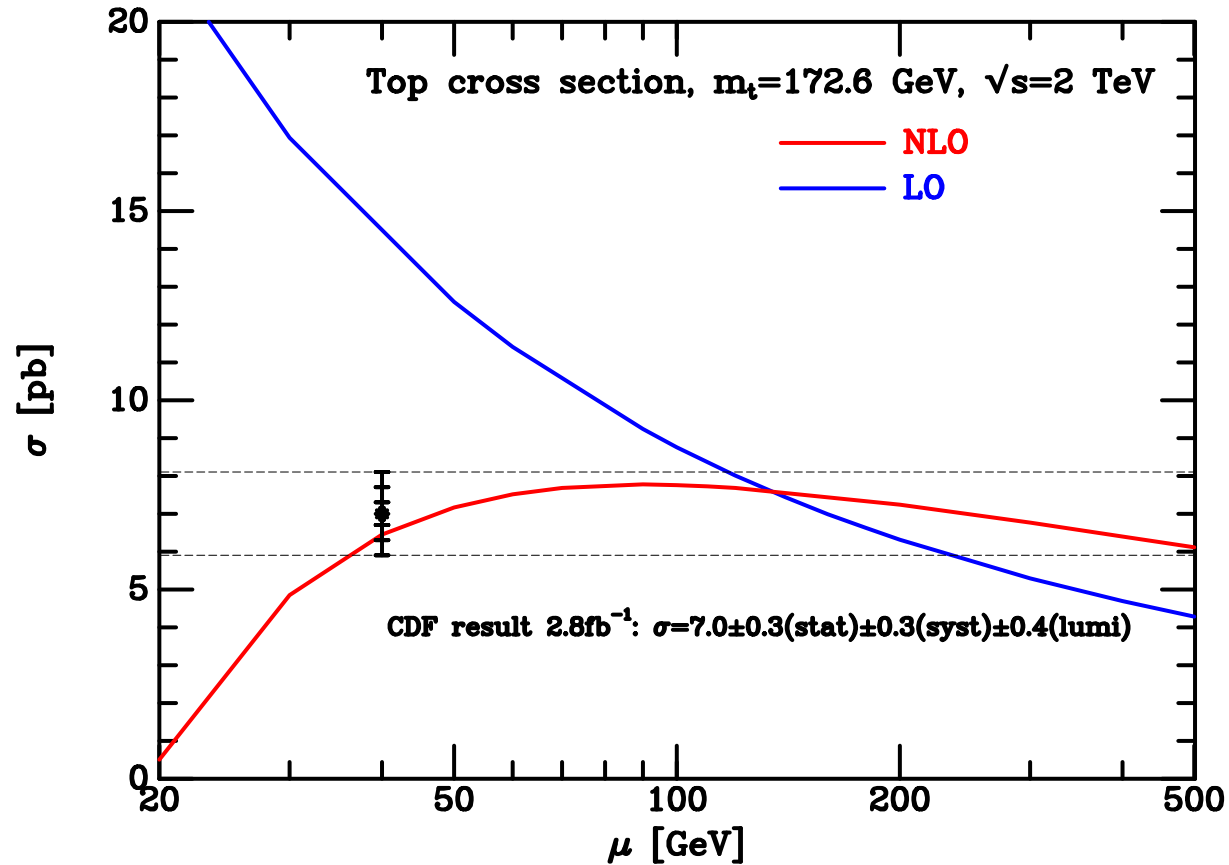
and the lowest-order form of the GLAP equation

$$\mu^2 \frac{d}{d\mu^2} f_i(x, \mu^2) = \frac{\alpha_S(\mu^2)}{2\pi} \sum_k \int_x^1 \frac{dz}{z} P_{ik}^{(0)}(z) f_k\left(\frac{x}{z}, \mu^2\right) + \dots$$

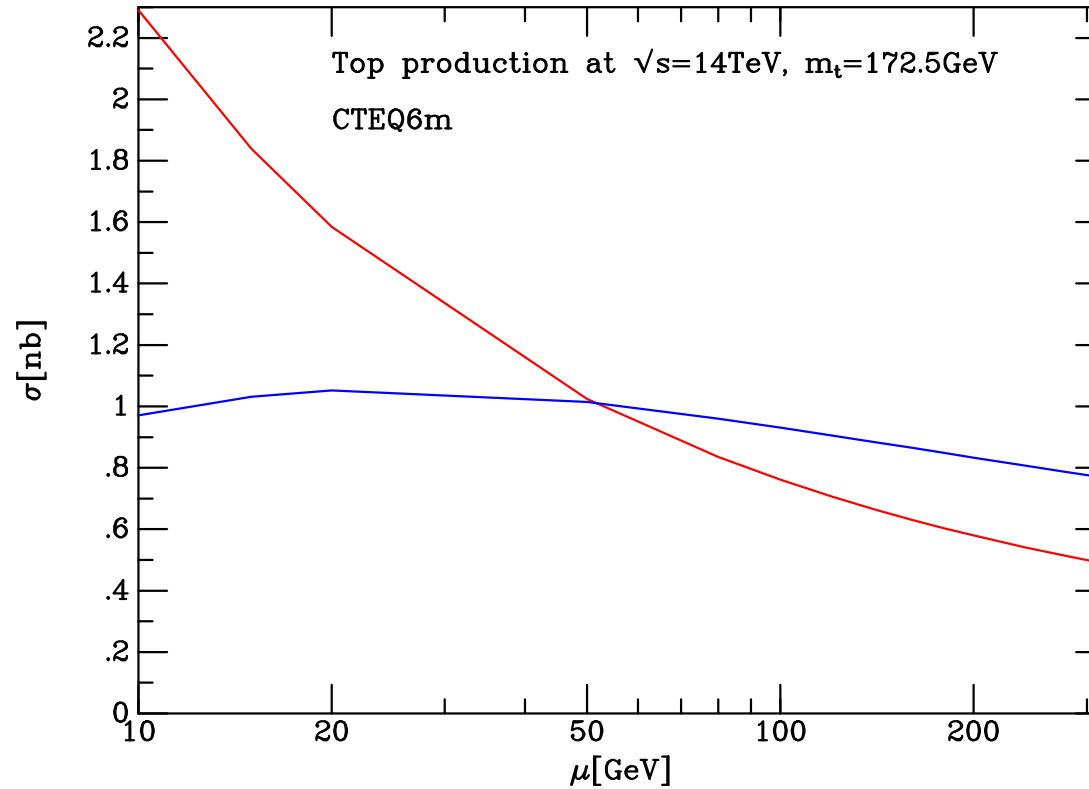
This illustrates an important point which is a general feature of renormalization group improved perturbation series in QCD. The coefficient of the perturbative correction depends on the choice made for the scale μ , but the scale dependence changes the result in such a way that the physical result is independent of that choice. Thus the scale dependence is formally small because it is of higher order in α_S . This does not assure us that the scale dependence is actually *numerically* small for all series. A pronounced dependence on the scale μ is a signal of an untrustworthy perturbation series.

Scale dependence in top production

- Inclusion of the higher order terms leads to a stabilization of the top cross section.



Top production at LHC



- At LHC top cross section is more than 100 times bigger than at Tevatron.

NLO QCD: Parton level integrators

- We would like to go beyond the results for the total cross section to get results for distributions.
- We have two separate divergent integrals which must be combined before numerical integration

$$\sigma_{NLO} = \int_{m+1} d\sigma^R + \int_m d\sigma^V$$

- Note that the jet definition can be arbitrarily complicated.

$$d\sigma^R = PS_{m+1} |\mathcal{M}_{m+1}|^2 F_{m+1}^J(p_1, \dots, p_{m+1})$$

We need to combine without knowledge of F^J .

- Two solutions: phase space slicing and subtraction.
- Illustrate with a simple one-dimensional example.

$$|\mathcal{M}_{m+1}|^2 \equiv \frac{1}{x} \mathcal{M}(x)$$

x is the energy of an emitted gluon.

- Divergences regularized in $d = 4 - 2\epsilon$ dimensions. Two solutions: phase space slicing and subtraction.
- Thus the full cross section in d dimensions is

$$\sigma = \int_0^1 \frac{dx}{x^{1+\epsilon}} \mathcal{M}(x) F_1^J(x) + \frac{1}{\epsilon} \nu F_0^J$$

- Infrared safety: $F_1^J(0) = F_0^J$, KLN cancellation theorem, $\mathcal{M}(0) = \nu$

Phase space slicing

- Introduce arbitrary cutoff $\delta \ll 1$

$$\sigma = \int_0^\delta \frac{dx}{x^{1+\epsilon}} \mathcal{M}(x) F_1^J(x) + \int_\delta^1 \frac{dx}{x^{1+\epsilon}} \mathcal{M}(x) F_1^J(x) + \frac{1}{\epsilon} \nu F_0^J \quad (1)$$

$$\simeq \int_0^\delta \frac{dx}{x^{1+\epsilon}} \nu F_0^J + \int_\delta^1 \frac{dx}{x} \mathcal{M}(x) F_1^J(x) + \frac{1}{\epsilon} \nu F_0^J \quad (2)$$

$$= \int_\delta^1 \frac{dx}{x} \mathcal{M}(x) F_1^J(x) + \ln(\delta) \nu F_0^J \quad (3)$$

(4)

- Procedure becomes exact for $\delta \rightarrow 0$ but numerical errors blow up. We have to compromise to find the best value of δ .
- Systematized by Giele-Glover-Kosower, JETRAD, DYRAD, EERAD

Subtraction method

■ Exact identity

$$\sigma = \int_0^1 \frac{dx}{x^{1+\epsilon}} \left[\mathcal{M}(x) F_1^J(x) - \mathcal{M}(0) F_0^J \right] + \int_0^1 \frac{dx}{x^{1+\epsilon}} \nu F_0^J + \frac{1}{\epsilon} \nu F_0^J \quad (5)$$

$$= \int_0^1 \frac{dx}{x} \left[\mathcal{M}(x) F_1^J(x) - \mathcal{M}(0) F_0^J \right] + O(1) \nu F_0^J \quad (6)$$

- We have divided the problem into two separately finite integrals.
- Subtracted cross section must be valid everywhere in phase space.
- Subtraction method used in NLOJET++, MCFM

MCFM overview

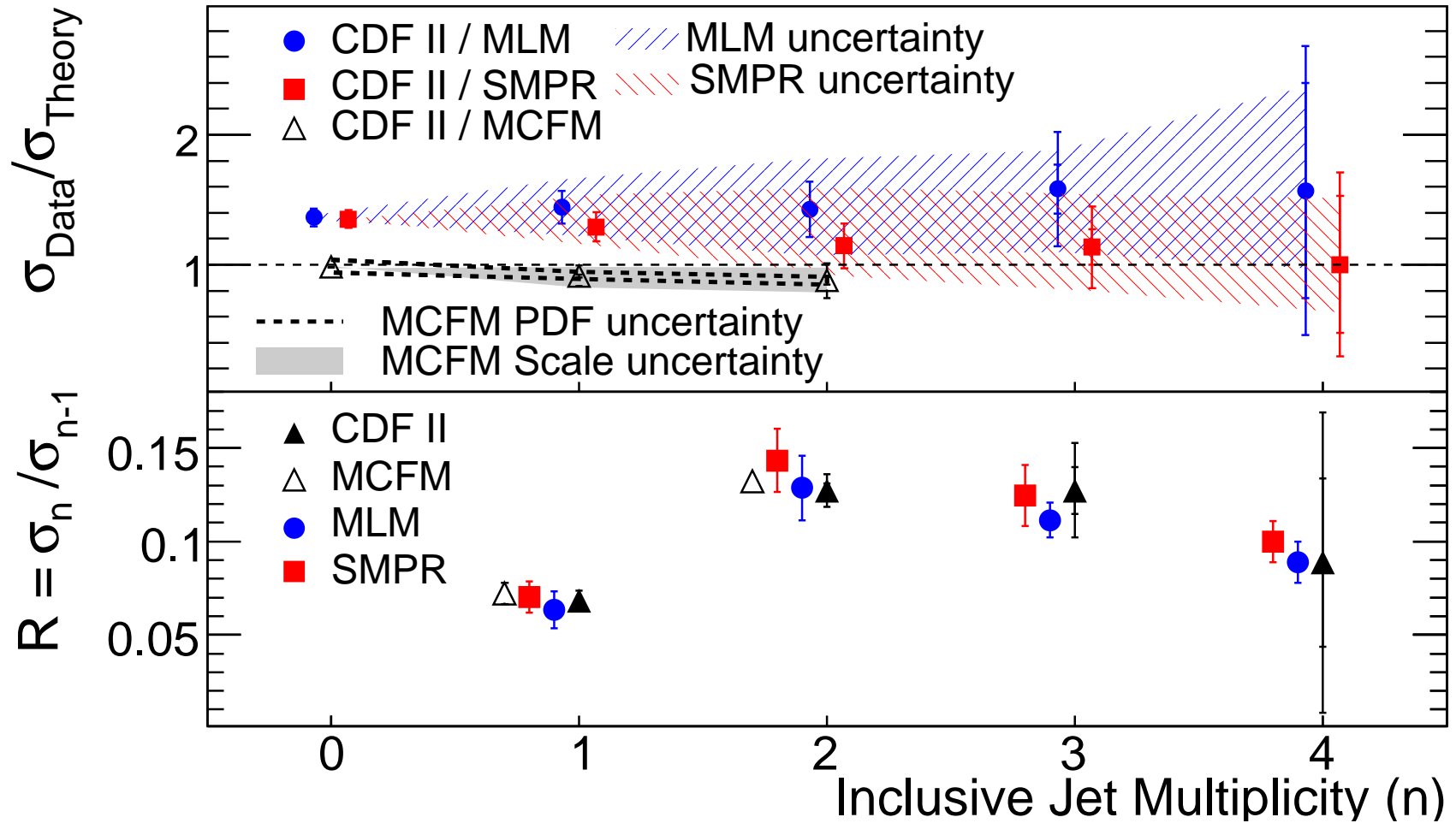
John Campbell and R.K. Ellis

- Parton level cross-sections predicted to NLO in α_S

$p\bar{p} \rightarrow W^\pm / Z$	$p\bar{p} \rightarrow W^+ + W^-$
$p\bar{p} \rightarrow W^\pm + Z$	$p\bar{p} \rightarrow Z + Z$
$p\bar{p} \rightarrow W^\pm + \gamma$	$p\bar{p} \rightarrow W^\pm / Z + H$
$p\bar{p} \rightarrow W^\pm + g^* (\rightarrow b\bar{b})$	$p\bar{p} \rightarrow Z b\bar{b}$
$p\bar{p} \rightarrow W^\pm / Z + 1 \text{ jet}$	$p\bar{p} \rightarrow W^\pm / Z + 2 \text{ jets}$
$p\bar{p}(gg) \rightarrow H$	$p\bar{p}(gg) \rightarrow H + 1 \text{ jet}$
$p\bar{p}(VV) \rightarrow H + 2 \text{ jets}$	$p\bar{p} \rightarrow t + X$
$pp \rightarrow t + W$	

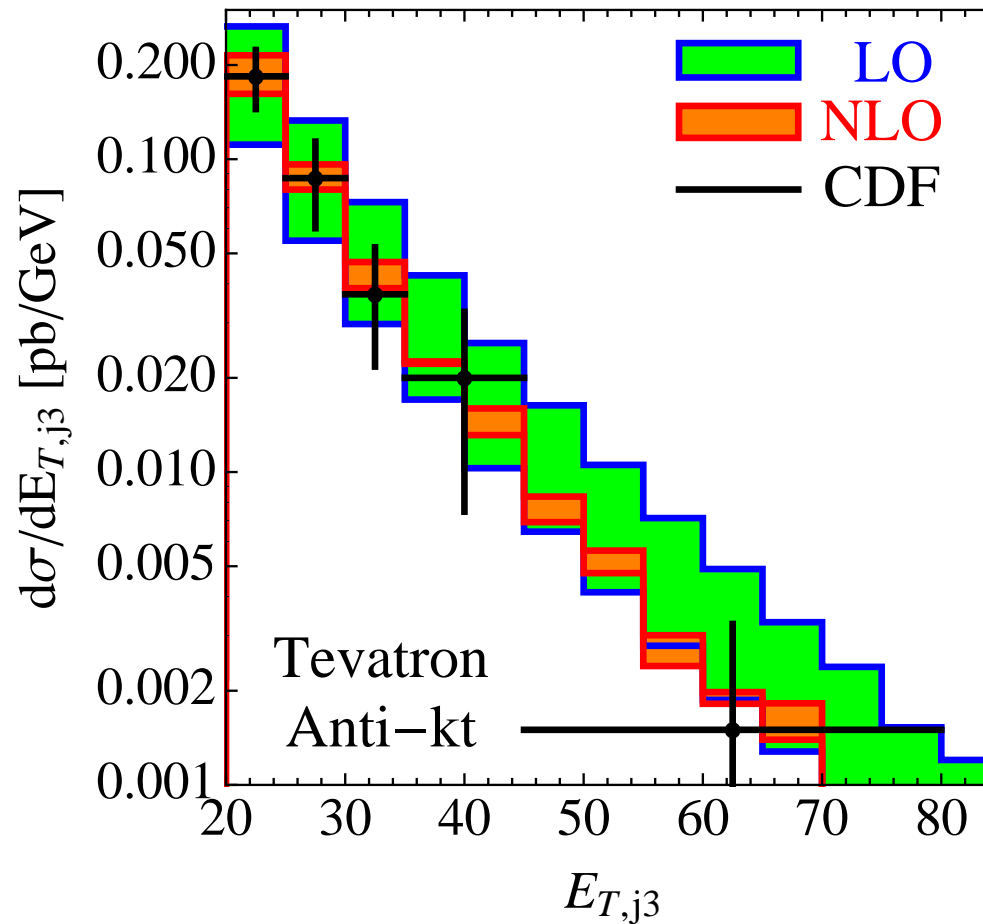
- ⊕ less sensitivity to μ_R, μ_F , rates are better normalized, fully differential distributions.
- ⊖ low particle multiplicity (no showering), no hadronization, hard to model detector effects
- ★ Based on the subtraction method

W + jet production



- Data is in agreement NLO prediction from MCFM
- Errors on tree level predictions (Alpgen+Herwig+MLM merging) and (Madgraph+Pythia+CKKW jet merging) are much larger.

New results on $W + 3\text{-jet}$ production



- Leading color results, arXiv:0906.1445v1
- CDF Data is in agreement NLO prediction from MCFM

Matching parton shower and NLO calculations

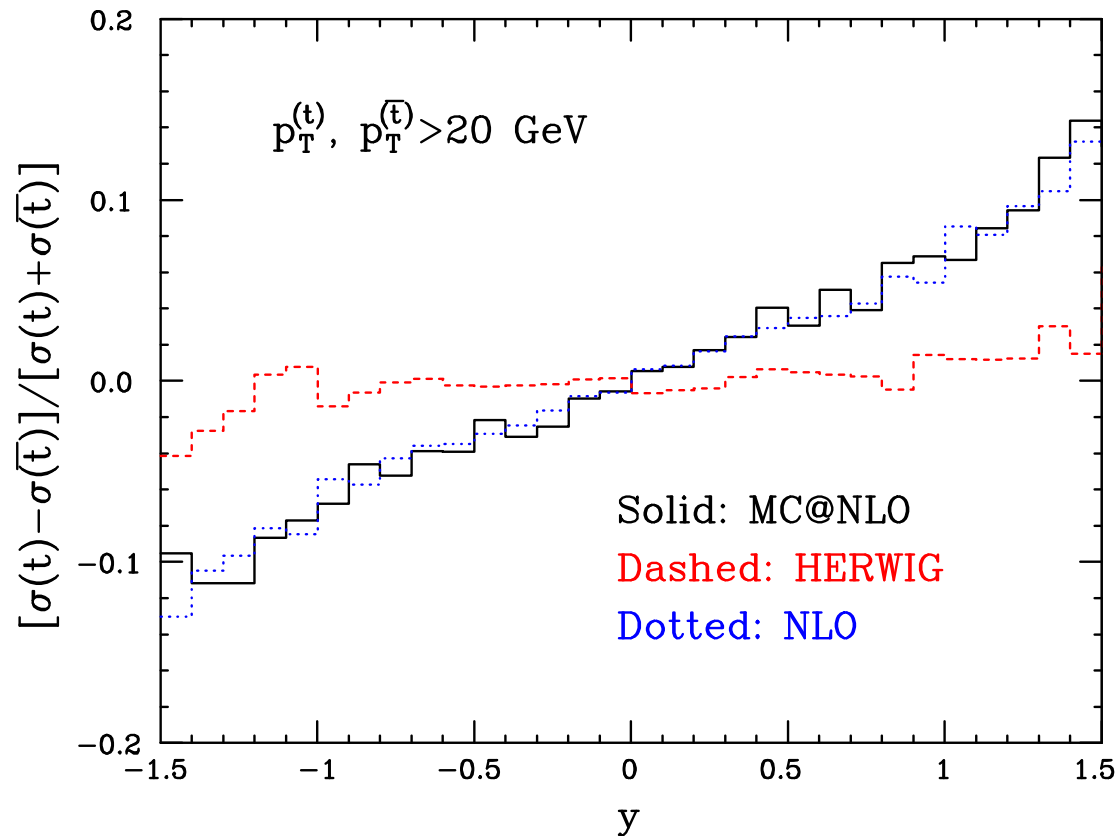
There are two methods for matching parton showers to NLO matrix elements, without double counting.

- MC@NLO method (Small number of negative weights)
 - ★ Frixione and Webber, JHEP 06 (2002) 029
- POWHEG method (only positive weights)
 - ★ Nason and Ridolfi JHEP 08 (2006) 077
 - ★ Frixione, Nason and Ridolfi, arXiv:0707.3088
 - ★ Frixione, Nason and Oleari, arXiv:0709.2092
- The method gives a result which when expanded to NLO is identical with the fixed order result, but also includes the parton shower.

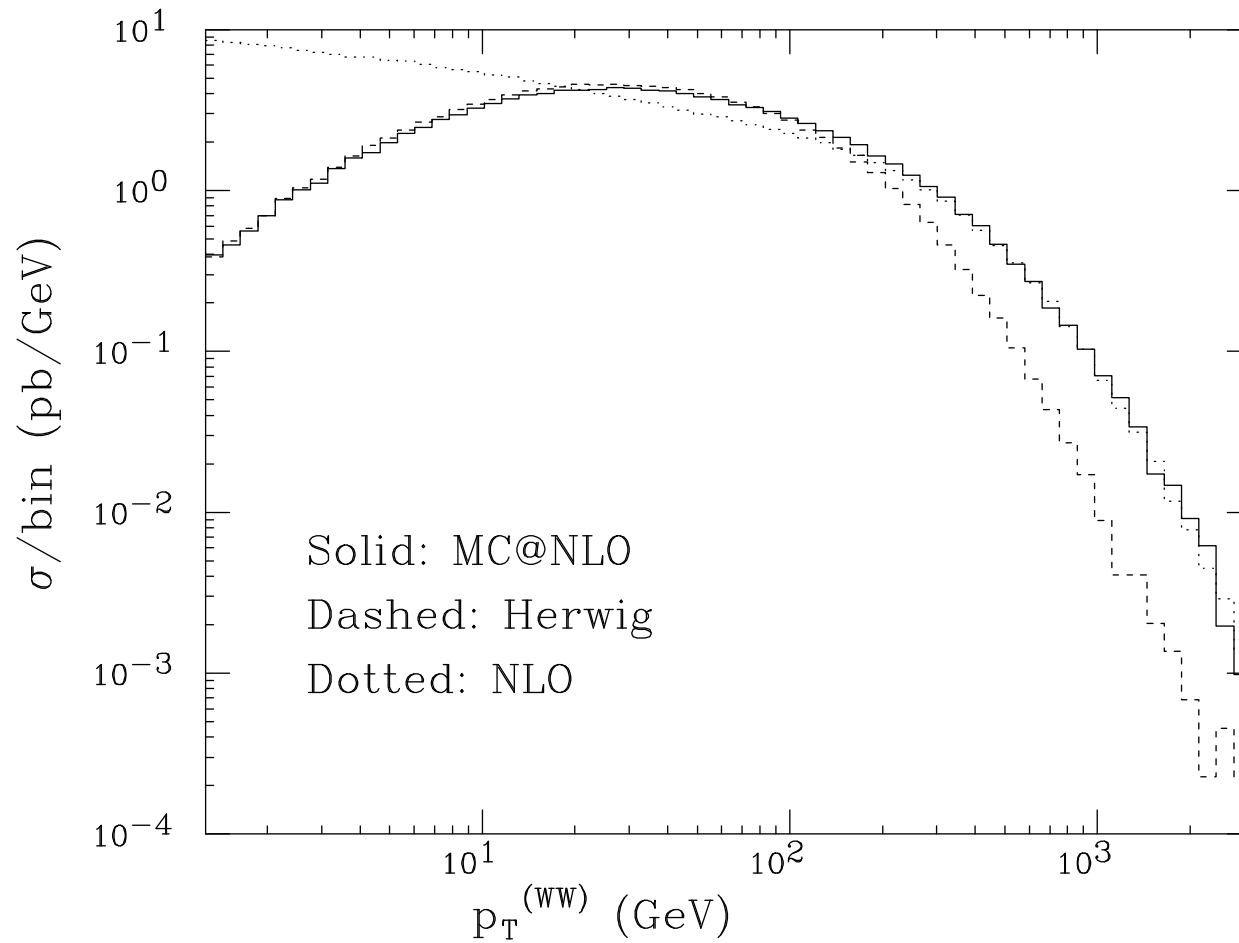
Asymmetry in top production

Frixione, Nason, Webber

- Example of $t\bar{t}$ -production using MC@NLO
- NLO curve (in blue, dotted).



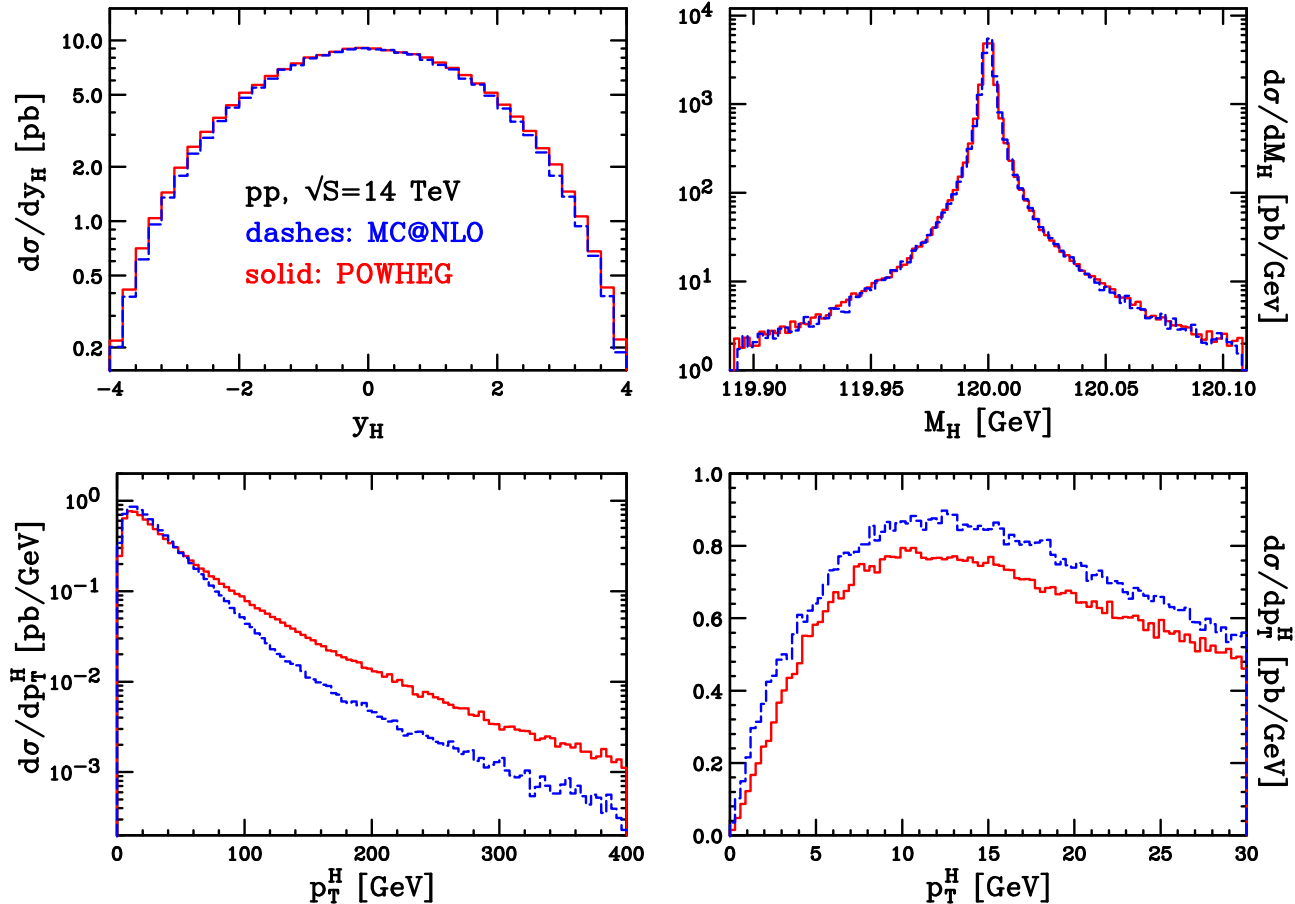
MC@NLO results



- Interpolates between MC and NLO in p_T^{WW}

POWHEG results on Higgs production

■ Example of H -production using POWHEG



■ Differences between POWHEG and MC@NLO are due to the implicit inclusion of differing non-leading logarithmic terms at NNLO.

■ Formula agree at NLO.

Conclusions

- NLO formulation of QCD processes gives better information about normalization, and less dependence on unphysical scales.
- Residual scale dependence can give an estimate of the size of the uncalculated higher order terms.
- NLO is hence the first serious approximation in QCD.
- NLO calculation can be performed using the subtraction or slicing method to give information about distributions.
- Many simple processes have been included at NLO in a unified framework (MCFM).
- For a limited (but ever growing) number of processes one can have both parton showers and NLO included in a consistent way.