1. Partonic cross sections

At the heart of the prediction of any hadron collider observable lies the calculation of the relevant hard scattering process. In this section we will outline the perturbative approaches that are employed to calculate these processes and describe some of their features and limitations. In addition, we will describe how the partonic calculations can be used to make predictions for an exclusive hadronic final state.

2. Lowest order calculations

The simplest predictions can be obtained by calculating the lowest order in the perturbative expansion of the observable, as discussed in the previous section. This is performed by calculating the squared matrix element represented by tree-level Feynman diagrams and integrating this over the appropriate phase space. For the simplest cases and for certain observables only, the phase space integration can be performed analytically. For example, in Section 2, we calculated the lowest order cross section for Drell-Yan production. However, to obtain fully differential predictions in general, the integration must be carried out numerically. For most calculations, it is necessary to impose restrictions on the phase space in order that divergences in the matrix elements are screened. This can best be understood by consideration of one of the simplest such cases, $W + 1$ jet production at a hadron collider.

2.1. $W + 1$ jet production

In Figure 1, we have extended the LO diagrams for Drell-Yan production by adding a final state gluon to each of the initial state quark legs. This is one of the subprocesses responsible for $W + 1$ jet production, with the other being $gq \rightarrow Wq$. After application of the Feynman rules, the squared matrix elements obtained from the sum of the diagrams take the form:

$$|M_{ud-W+g}|^2 \sim \left( \frac{\hat{t}^2 + \hat{u}^2 + 2Q^2 \hat{s}}{\hat{t}\hat{u}} \right), \quad (1)$$
where $Q^2$ is the virtuality of the $W$ boson, $\hat{s} = s_{ud}$, $\hat{t} = s_{ug}$, and $\hat{u} = s_{\bar{d}g}$, c.f. Equation (22) of Section 2. This expression diverges in the limit where the gluon is unresolved – either it is collinear to one of the quarks ($\hat{t} \to 0$ or $\hat{u} \to 0$), or it is soft (both invariants vanish, so $E_g \to 0$). Let us consider the impact of these divergences on the calculation of this cross section. In order to turn the matrix elements into a cross section, one must convolute with PDF’s and perform the integration over the appropriate phase space,

$$\sigma = \int dx_1 dx_2 f_u(x_1, Q^2) f_{\bar{d}}(x_2, Q^2) \frac{|M|^2}{32\pi^2} \frac{d^3p_W}{E_W} \frac{d^3p_g}{E_g} \delta(p_u + p_{\bar{d}} - p_W - p_g), (2)$$

where $x_1, x_2$ are the momentum fractions of the $u$ and $\bar{d}$ quarks. These momentum fractions are of course related to the centre of mass energy of the collider $s$ by the relation, $\hat{s} = x_1 x_2 s$.

After suitable manipulations, this can be transformed into a cross-section that is differential in $Q^2$ and the transverse momentum ($p_T$) and rapidity ($y$) of the $W$ boson [24],

$$\frac{d\sigma}{dQ^2 dy dp_T^2} \sim \frac{1}{s} \int dy_g f_u(x_1, Q^2) f_{\bar{d}}(x_2, Q^2) \frac{|M|^2}{\hat{s}}$$

The remaining integral to be done is over the rapidity of the gluon, $y_g$. Note that the $p_T$ of the gluon is related to the invariants of the process by $p_T^2 = \hat{t} \hat{u} / \hat{s}$, so that the leading divergence represented by the third term of Equation 1 corresponds to the limit $p_T \to 0$. Furthermore, in this limit $\hat{s} \to Q^2$, so that the behaviour of the cross-section becomes,

$$\frac{d\sigma}{dQ^2 dy dp_T^2} \sim \frac{1}{s} \frac{1}{p_T^2} \int dy_g f_u(x_1, Q^2) f_{\bar{d}}(x_2, Q^2) + \text{sub-leading in } p_T^2$$

(4)

As the $p_T$ of the $W$ boson becomes small, the limits on the $y_g$ integration are given by $\pm \log(\sqrt{s}/p_T)$. Under the assumption that the rest of the integrand is approximately constant, the integral can be simply performed. This yields,

$$\frac{d\sigma}{dQ^2 dy dp_T^2} \sim \frac{\log(s/p_T^2)}{p_T^2},$$

so that the differential cross section contains a logarithmic dependence on $p_T$. If no cut is applied on the gluon $p_T$ we see that this result makes no sense – only after applying a minimum value of the $p_T$ do we obtain a finite result. However, applying a cutoff at $p_T = p_{T,\text{min}}$ and then performing the integration yields a result proportional to $\log^2(s/p_{T,\text{min}}^2)$. This is typical of a fixed order expansion – it is not merely an expansion in $\alpha_s$, but in $\alpha_s \log(\ldots)$, where the argument of the logarithm depends upon the process and cuts under consideration. As we shall discuss later, these logarithms may be systematically accounted for in various all-orders treatments.

In Figure 2 we show the the rapidity distribution of the jet, calculated using this lowest order process. In the calculation, a sum over all species of quarks has been performed and the contribution from the quark-gluon process included. The rapidity distribution is shown for two different choices of minimum jet transverse momentum,
Figure 2. The rapidity distribution of the final state parton found in a lowest order calculation of the $W + 1$ jet cross section at the LHC. The parton is required to have a $p_T$ larger than 2 GeV (left) or 50 GeV (right). Contributions from $q\bar{q}$ annihilation (solid red line) and the $qg$ process (dashed blue line) are shown separately.

which is the cut-off used to regulate the collinear divergences discussed above. For very small values of $p_T$, we can view the radiated gluon as being emitted from the quark line at an early time, typically termed “initial-state radiation”. From the left-hand plot, this radiation is indeed produced quite often at large rapidities, although it is also emitted centrally with a large probability. The canonical “wisdom” is that initial-state radiation is primarily found in the forward region. There is indeed a collinear pole in the matrix element so that a fixed energy gluon tends to be emitted close to the original parton direction. However, we are interested not in fixed energy but rather in fixed transverse momentum. When using a higher $p_T$ cut-off the gluon is emitted less often at large rapidities and is more central, as shown by the plot on the right-hand side. In this case, one can instead think of the diagrams as a $2 \rightarrow 2$ scattering as depicted in Figure 3. Of course, the manner in which such Feynman diagrams are drawn is purely a matter of convention. The diagrams are exactly the same as in Figure 1, but re-drawing them in this way is suggestive of the different kinematic region that is probed with a gluon at high $p_T$.

There is also a collinear pole involved for the emission of gluons from final state partons. Thus, the gluons will be emitted preferentially near the direction of the emitting parton. In fact, it is just such emissions that give rise to the finite size of the jet arising
from a single final state parton originating from the hard scatter. Much of the jet structure is determined by the hardest gluon emission; thus NLO theory, in which a jet consists of at most 2 partons, provides a good description of the jet shape observed in data [1].

2.2. \( W + 2 \) jet production

By adding a further parton, one can simulate the production of a \( W + 2 \) jet final state. Many different partonic processes contribute in general, so for the sake of illustration we just consider the production of a \( W \) boson in association with two gluons.

First, we shall study the singularity structure of the matrix elements in more detail. In the limit that one of the gluons, \( p_1 \) is soft, the singularities in the matrix elements occur in 4 diagrams only. These diagrams, in which gluon \( p_1 \) is radiated from an external line, are depicted in Figure 4. The remaining diagrams, in which gluon \( p_1 \) is attached to an internal line, do not give rise to singularities because the adjacent propagator does not vanish in this limit.

This is the first of our examples in which the matrix elements contain non-trivial colour structure. Denoting the colour labels of gluons \( p_1 \) and \( p_2 \) by \( t^A \) and \( t^B \) respectively, diagram (1) is proportional to \( t^B t^A \), whilst (2) is proportional to \( t^A t^B \). The final two diagrams, (3a) and (3b) are each proportional to \( f^{ABC} t^C \), which can of course be written as \( (t^A t^B - t^B t^A) \). Using this identity, the amplitude (in the limit that \( p_1 \) is soft) can be written in a form in which the dependence on the colour matrices is factored out,

\[
\mathcal{M}^{q\bar{q}\rightarrow Wgg} = t^A t^B (D_2 + D_3) + t^B t^A (D_1 - D_3)
\]

so that the the kinematic structures obtained from the Feynman rules are collected in

Figure 4. The 4 diagrams that contribute to the matrix elements for the production of \( W + 2 \) gluons when gluon 1 is soft.
the functions $D_1$, $D_2$ (for diagrams (1) and (2)) and $D_3$ (the sum of diagrams (3a) and (3b)). The combinations that appear in equation 6 are often referred to as colour-ordered amplitudes.

With the colour factors stripped out, it is straightforward to square the amplitude in equation 6 using the identities $\text{tr}(t^A t^B t^A t^B) = N C_F^2$ and $\text{tr}(t^A t^B t^A) = -C_F/2$,

$$|\mathcal{M}^{q\bar{q} \rightarrow Wgg}|^2 = N C_F^2 \left[ |D_2 + D_3|^2 + |D_1 - D_3|^2 \right] - C_F (D_2 + D_3)(D_1 - D_3)^\dagger$$

$$= \frac{C_F N^2}{2} \left[ |D_2 + D_3|^2 + |D_1 - D_3|^2 - \frac{1}{N^2} |D_1 + D_2|^2 \right]. \quad (7)$$

Moreover, these colour-ordered amplitudes possess special factorization properties in the limit that gluon $p_1$ is soft. In this limit they can be written as the product of an eikonal term and the matrix elements containing only one gluon,

$$D_2 + D_3 \rightarrow \epsilon_{\mu} \left( \frac{q^\mu}{p_1.q} - \frac{p_2^\mu}{p_1.p_2} \right) \mathcal{M}_{q\bar{q} \rightarrow Wg}$$

$$D_1 - D_3 \rightarrow \epsilon_{\mu} \left( \frac{p_2^\mu}{p_1.p_2} - \frac{\bar{q}^\mu}{p_1.\bar{q}} \right) \mathcal{M}_{q\bar{q} \rightarrow Wg} \quad (8)$$

where $\epsilon_{\mu}$ is the polarization vector for gluon $p_1$. The squares of these eikonal terms are easily computed using the replacement $\epsilon_{\mu} \epsilon^*_{\nu} \rightarrow -g_{\mu\nu}$ to sum over the gluon polarizations. This yields terms of the form,

$$\frac{a.b}{p_1.a p_1.b} \equiv [a b], \quad (9)$$

so that the final result is,

$$|\mathcal{M}^{q\bar{q} \rightarrow Wgg}|^2 \xrightarrow{\text{soft}} \frac{C_F N^2}{2} \left[ [q p_2] + [p_2 \bar{q}] - \frac{1}{N^2} [q \bar{q}] \right] \mathcal{M}^{q\bar{q} \rightarrow Wg}. \quad (10)$$

Inspecting this equation, one can see that the leading term (in the number of colours) contains singularities along two lines of colour flow – one connecting the gluon $p_2$ to the quark, the other connecting it to the anti-quark. On the other hand, the sub-leading term has singularities along the line connecting the quark and anti-quark. It is these lines of colour flow that indicate the preferred directions for the emission of additional gluons. In the sub-leading term the colour flow does not relate the gluon colour to the parent quarks at all. The matrix elements are in fact the same as those for the emission of two photons from a quark line (apart from overall coupling factors) with no unique assignment to either diagram 1 or diagram 2, unlike the leading term. For this reason only the information about the leading colour flow is used by parton shower Monte Carlos such as Herwig and Pythia. As a further example, the lines of colour flow in a $W + 2$ jet event are shown in Figure 5.

Since all the partons are massless, it is trivial to re-write the eikonal factor of equation 9 in terms of the energy of the radiated gluon, $E$ and the angle it makes with the hard partons, $\theta_a, \theta_b$. It can then be combined with the phase space for the emitted gluon to yield a contribution such as,

$$[a b] dP S_{\text{gluon}} = \frac{1}{E^2} \frac{1}{1 - \cos \theta_a} E dE d \cos \theta_a. \quad (11)$$
In this form, it is clear that the cross-section diverges as either \( \cos \theta_a \to 1 \) (the gluon is emitted collinear to parton \( a \)) or \( E \to 0 \) (for any angle of radiation). Moreover, each divergence is logarithmic and regulating the divergence, by providing a fixed cutoff (either in angle or energy) will produce a single logarithm from collinear configurations and another from soft ones — just as we found when considering the specific case of \( W + 1 \) jet production in the previous subsection.

This argument can be applied at successively higher orders of perturbation theory. Each gluon that is added yields an additional power of \( \alpha_s \) and, via the eikonal factorization outlined above, can produce an additional two logarithms. This means that we can write the \( W + 1 \) jet cross section schematically as a sum of contributions,

\[
d\sigma = \sigma_0(W + 1 \text{ jet}) \left[ 1 + \alpha_s (c_{12} L^2 + c_{11} L + c_{10}) + \alpha_s^2 (c_{24} L^4 + c_{23} L^3 + c_{22} L^2 + c_{21} L + c_{20}) + \ldots \right] \tag{12}
\]

where \( L \) represents the logarithm controlling the divergence, either soft or collinear. The size of \( L \) depends upon the criteria used to define the jets — the minimum transverse energy of a jet and the jet cone size. The coefficients \( c_{ij} \) in front of the logarithms depend upon colour factors (and ???). Note that the addition of each gluon results not just in an additional factor of \( \alpha_s \), but in a factor of \( \alpha_s \) times logarithms. For many important kinematic configurations, the logs can be large, leading to an enhanced probability for additional gluon emissions to occur. For inclusive quantities, where the same cuts are applied to every jet, the logs tends to be small, and counting powers of \( \alpha_s \) becomes a valid estimator for the rate of production of additional jets.

Noticing that the factor \( (\alpha_s L) \) appears throughout Equation 12, it is useful to re-write the expansion in brackets as,

\[
[\ldots] = 1 + \alpha_s L^2 c_{12} + (\alpha_s L^2)^2 c_{24} + \alpha_s L c_{11} (1 + \alpha_s L^2 c_{23}/c_{11} + \ldots) + \ldots \\
= \exp \left[ c_{12} \alpha_s L^2 + c_{11} \alpha_s L \right], \tag{13}
\]

where the infinite series have been resummed into an exponential form. The first term in the exponent is commonly referred to as the leading logarithmic term, with the second being required in order to reproduce next-to-leading logarithms. This reorganization of the perturbative expansion is especially useful when the product \( \alpha_s L \) is large, for
Figure 6. A final state configuration containing a $W$ and 2 partons. After the jet definition has been applied, either zero, one or two jets may be reconstructed.

instance when the logarithm is a ratio of two physical scales that are very different such as $\log(m_H/m_b)$. This exponential form is the basis of all orders predictions and can be interpreted in terms of Sudakov probabilities, both subjects that we will return to in later discussions.

It is instructive to recast the discussion of the total $W$ cross section in these terms, where the calculation is decomposed into components that each contain a given number of jets:

$$\sigma_W = \sigma_{W+0j} + \sigma_{W+1j} + \sigma_{W+2j} + \sigma_{W+3j} + \ldots \quad (14)$$

Now, as in equation 12, we can further write out each contribution as an expansion in powers of $\alpha_s$ and logarithms,

$$\sigma_{W+0j} = a_0 + \alpha_s(a_{12}L^2 + a_{11}L + a_{10}) + \alpha_s^2(a_{24}L^4 + a_{23}L^3 + a_{22}L^2 + a_{21}L + a_{20}) + \ldots$$

$$\sigma_{W+1j} = \alpha_s(b_{12}L^2 + b_{11}L + b_{10}) + \alpha_s^2(b_{24}L^4 + b_{23}L^3 + b_{22}L^2 + b_{21}L + b_{20}) + \ldots$$

$$\sigma_{W+2j} = \ldots \quad (15)$$

As the jet definitions change, the size of the logarithms shuffle the contributions from one term to another. For example, as the jet cone size is decreased the logarithm $L$ increases. As a result, the average jet multiplicity goes up and terms in Equation 14 that represent relatively higher multiplicities will become more important.

This is illustrated in Figure 6. Such a configuration may be reconstructed as an event containing up to two jets, depending upon the jet definition and the momenta of the partons. The matrix elements for this process contain terms proportional to $\alpha_s \log(p_{T,3}/p_{T,4})$ and $\alpha_s \log(1/\Delta R_{34})$ which is the reason that minimum values for the transverse energy and separation must be imposed. We shall see later that this is not the case at next-to-leading order.
Finally, we note that although the decomposition in equation 14 introduces quantities which are dependent upon the jet definition, we can recover results that are independent of these parameters by simply summing up the terms in the expansion that enter at the same order of perturbation theory. In this way, we just recover the perturbative expansion of the total cross section,

\[
\sigma_{LO} = a_0 \\
\sigma_{NLO} = \alpha_s \left( a_{12} L^2 + a_{11} L + a_{10} + b_{12} L^2 + b_{11} L + b_{10} \right).
\]

2.3. Leading order tools

Once suitable cuts have been applied, as we have discussed extensively above, leading order cross sections can be calculated using a number of computer programs.

There is a wide range of programs available, most notably ALPGEN [2, 3], the COMPHEP package [4, 5] and Madgraph [6, 7]. All of these programs implement the calculation of the diagrams numerically and provide a suitable phase space over which they can be integrated. ALPGEN uses an approach which is not based on a traditional Feynman diagram evaluation [8], whereas the other two programs rely on more conventional methods such as the helicity amplitudes evaluation of HELAS [9] in Madgraph.

Although in principle these programs can be used to calculate any tree-level prediction, in practice the complexity of the process that may be studied is limited by the number of particles that is produced in the final state. This is largely due to the factorial growth in the number of Feynman diagrams that must be calculated. Even in approaches which do not rely directly on the Feynman diagrams, the growth is still as a power of the number of particles. For processes which involve a large number of quarks and gluons, as is the case when attempting to describe a multi-jet final state at a hadron collider such as the Tevatron or the LHC, an additional concern is the calculation of colour matrices which appear as coefficients in the amplitudes [10].

In many cases, such as in the calculation of amplitudes representing multiple gluon scattering, the final result is remarkably simple. Motivated by such results, the last couple of years has seen remarkable progress in the development of new approaches to QCD tree-level calculations. Some of the structure behind the amplitudes can be understood by transforming to “twistor space” [11], in which amplitudes are represented by intersecting lines. This idea can be taken further with the introduction of “MHV” rules [12], which use the simplest (maximally helicity-violating, or MHV) amplitudes as the building blocks of more complicated ones. Although these rules at first only applied to amplitudes containing gluons, they were soon extended to cases of more general interest at hadron colliders [13, 14, 15, 16, 17, 18]. Even more recently, further simplification of amplitudes has been obtained by using “on-shell recursion relations” [19, 20]. As well as providing very compact expressions, this approach has the advantage of being both easily proven and readily extendible to processes involving fermions and vector bosons.
3. Next-to-leading order calculations

Although lowest order calculations can in general describe broad features of a particular process and provide the first estimate of its cross section, in many cases this approximation is insufficient. The inherent uncertainty in a lowest order calculation derives from its dependence on the unphysical renormalization and factorization scales, which is often large. In addition, some processes may contain large logarithms that need to be resummed or extra partonic processes may contribute only when going beyond the first approximation. Thus, in order to compare with predictions that have smaller theoretical uncertainties, next-to-leading order (NLO) calculations are imperative for experimental analyses in Run II of the Tevatron and at the LHC.

3.1. Virtual and real radiation contributions

A next-to-leading order QCD calculation requires the consideration of all diagrams that contribute an additional strong coupling factor, $\alpha_s$. These diagrams are obtained from the lowest order ones by adding additional quarks and gluons and they can be divided into two categories, virtual (or loop) contributions and the real radiation component. We shall illustrate this by considering the next-to-leading order corrections to Drell-Yan production at a hadron collider. The virtual diagrams for this process are shown in Figure 7 whilst the real diagrams are exactly the ones that enter the $W + 1$ jet calculation (in Figure 1).

Let us first consider the virtual contributions. In order to evaluate the diagrams in Figure 7, it is necessary to introduce an additional loop momentum $\ell$ which circulates around the loop in each diagram and is unconstrained. To complete the evaluation of these diagrams, one must therefore integrate over the momentum $\ell$. However, the resulting contribution is not finite but contains infrared divergences – in the same way that the diagrams of Figure 1 contain infrared (soft and collinear) singularities. By isolating the singularities appropriately, one can see that the divergences that appear in each contribution are equal, but of opposite sign. The fact that the sum is finite is a demonstration of the theorems of Bloch and Nordsieck [21] and Kinoshita, Lee and Nauenberg [22, 23], which guarantee that this is the case at all orders in perturbation
theory and for any number of final state particles.

The real contribution consists of the diagrams in Figure 1, together with a quark-gluon scattering piece that can be obtained from these diagrams by interchanging the gluon in the final state with a quark (or antiquark) in the initial state. As discussed in the previous section, the quark-antiquark matrix elements contain a singularity as the gluon transverse momentum vanishes.

In our NLO calculation we want to carefully regulate and then isolate these singularities in order to extend the treatment down to zero transverse momentum. The most common method to regulate the singularities is dimensional regularization. In this approach, the number of dimensions is continued to $D = 4 - 2\epsilon$ so that in intermediate stages the singularities appear as single and double poles in $\epsilon$. After they have cancelled, the limit $D \to 4$ can be safely taken. Within this scheme, the cancellation of divergences between real and virtual terms can be seen schematically by consideration of a toy calculation [25],

$$I = \lim_{\epsilon \to 0} \left( \int_0^1 \frac{dx}{x} x^\epsilon M(x) - \frac{1}{\epsilon} M(0) \right).$$

Here, $M(x)$ represents the real radiation matrix elements which are integrated over the extra phase space of the gluon emission, which contains a factor $x^\epsilon$. $x$ represents a kinematic invariant which vanishes as the gluon becomes unresolved. The second term is representative of the virtual contribution, which contains an explicit pole, $1/\epsilon$, multiplying the lowest order matrix elements, $M(0)$.

Two main techniques have been developed for isolating the singularities, which are commonly referred to as the subtraction method [26, 27, 28, 29] and phase-space slicing [30, 31]. For the sake of illustration, we shall consider only the subtraction method. In this approach, one explicitly adds and subtracts a divergent term such that the new real radiation integral is manifestly finite. In the toy integral this corresponds to,

$$I = \lim_{\epsilon \to 0} \left( \int_0^1 \frac{dx}{x} x^\epsilon [M(x) - M(0)] + M(0) \int_0^1 \frac{dx}{x} x^\epsilon - \frac{1}{\epsilon} M(0) \right)$$

$$= \int_0^1 \frac{dx}{x} [M(x) - M(0)].$$

This idea can be generalized in order to render finite the real radiation contribution to any process, with a separate counter-term for each singular region of phase space. Processes with a complicated phase space, such as $W+2$ jet production, can end up with a large number of counterterms. NLO calculations are often set up to generate cross sections by histogramming “events” generated with the relevant matrix elements. Such events can not be directly interfaced to parton shower programs as the presence of virtual corrections means that many of the events will have (often large) negative weights. Only the total sum of events over all relevant subprocesses will lead to a physically meaningful cross section.

The inclusion of real radiation diagrams in a NLO calculation extends the range of predictions that may be described by a lowest order calculation. For instance, in
the example above the $W$ boson is produced with zero transverse momentum at lowest order and only acquires a finite $p_T$ at NLO. Even then, the $W$ transverse momentum is exactly balanced by that of a single parton. In a real event, the $W$ $p_T$ is balanced by the sum of several jet transverse momenta. In a fixed order calculation, these contributions would be included by moving to even higher orders so that, for instance, configurations where the $W$ transverse momentum is balanced by two jets enter at NNLO. Although this feature is clear for the $p_T$ distribution of the $W$, the same argument applies for other distributions and for more complex processes.

### 3.2. Scale dependence

One of the benefits of performing a calculation to higher order in perturbation theory is the reduction of the dependence of related predictions on the unphysical renormalization ($\mu_R$) and factorization scales ($\mu_F$). This can be demonstrated by considering inclusive jet production from a quark anti-quark initial state [32], which is represented by the lowest order diagrams shown in Figure 8. This is a simplification of the full calculation, but is the dominant contribution when the typical jet transverse momentum is large.

For this process, we can write the lowest order prediction for the single jet inclusive distribution as,

$$
\frac{d\sigma}{dE_T} = \alpha_s^2(\mu_R) \sigma_0 \otimes f_q(\mu_F) \otimes f_{\bar{q}}(\mu_F),
$$

(18)

where $\sigma_0$ represents the lowest order partonic cross section calculated from the diagrams of Figure 8 and $f_i(\mu_F)$ is the parton distribution function for a parton $i$. Similarly, after including the next-to-leading order corrections, the prediction can be written as,

$$
\frac{d\sigma}{dE_T} = \left[ \alpha_s^2(\mu_R) \sigma_0 + \alpha_s^3(\mu_R) \left( \sigma_1 + 2 b_0 \log(\mu_R/E_T) \sigma_0 - 2 P_{qq} \log(\mu_F/E_T) \sigma_0 \right) \right] \\
\otimes f_q(\mu_F) \otimes f_{\bar{q}}(\mu_F).
$$

(19)

In this expression, the explicit logarithms involving the renormalization and factorization scales have been exposed. The remainder of the $O(\alpha_s^3)$ corrections lie in the function $\sigma_1$. 

**Figure 8.** The leading order diagrams representing inclusive jet production from a quark anti-quark initial state.
From this expression, the sensitivity of the distribution to the renormalization scale is easily calculated using,

\[ \mu_R \frac{\partial \alpha_s(\mu_R)}{\partial \mu_R} = -b_0 \alpha_s^2(\mu_R) - b_1 \alpha_s^3(\mu_R) + \mathcal{O}(\alpha_s^4), \]

(20)

where the two leading coefficients in the beta-function, \( b_0 \) and \( b_1 \), are given by \( b_0 = (33 - 2n_f)/6\pi \) and \( b_1 = (102 - 38n_f/3)/8\pi^2 \). The contributions from the first and third terms in equation (19) cancel and the result vanishes, up to \( \mathcal{O}(\alpha_s^4) \).

In a similar fashion, the factorization scale dependence can be calculated using the non-singlet DGLAP equation,

\[ \mu_F \frac{\partial f_i(\mu_F)}{\partial \mu_F} = \alpha_s(\mu_F) P_{qq} \otimes f_i(\mu_F). \]

(21)

This time, the partial derivative of each parton distribution function, multiplied by the first term in equation (19) cancels with the final term. Thus, once again, the only remaining terms are of order \( \alpha_s^4 \).

This is a generic feature of a next-to-leading order calculation. An observable that is predicted to order \( \alpha_s^3 \) is independent of the choice of either renormalization or factorization scale, up to the next higher order in \( \alpha_s \).

This discussion can be made more concrete by inserting numerical results into the formulae indicated above. For simplicity, we will consider only the renormalization scaled dependence, with the factorization scale held fixed at \( \mu_F = E_T \). In this case it is simple to extend equation (19) one higher order in \( \alpha_s \) [37],

\[ \frac{d\sigma}{dE_T} = \left[ \alpha_s^2(\mu_R) \sigma_0 + \alpha_s^3(\mu_R) \left( \sigma_1 + 2b_0 L \sigma_0 \right) \right. \]

\[ + \left. \alpha_s^4(\mu_R) \left( \sigma_2 + 3b_0 L \sigma_1 + (3b_0^2 L^2 + 2b_1 L) \sigma_0 \right) \right] \otimes f_q(\mu_F) \otimes f_{\bar{q}}(\mu_F), \]

where the logarithm is abbreviated as \( L \equiv \log(\mu_R/E_T) \). For a realistic example at the Tevatron Run I, \( \sigma_0 = 24.4 \) and \( \sigma_1 = 101.5 \). With these values the LO and NLO scale dependence can be calculated; the result is shown in Figure 9. At the moment the value of \( \sigma_2 \) is unknown (see the NNLO section below). However, a range of predictions based on plausible values that it could take are also shown in the figure, \( \sigma_2 = 0 \) (solid) and \( \sigma_2 = \pm \sigma_1^2/\sigma_0 \) (dashed). It is clear that the renormalization scale dependence is reduced when going from LO and NLO and will become smaller still at NNLO.

Although Figure 9 is representative of the situation found at NLO, the exact details depend upon the kinematics of the process under study and on choices such as the running of \( \alpha_s \) and the PDF’s used. Of particular interest are the positions on the NLO curve which correspond to often-used scale choices. Due to the structure of equation 19 there will always be a peak in the NLO curve, around which the scale dependence is minimized. The scale at which this peak occurs is often favoured as a choice. For example, for inclusive jet production at the Tevatron, a scale of \( E_T^{jet}/2 \) is usually chosen. This is near the peak of the NLO cross section for many kinematic regions. It is also usually near the scale at which the LO and NLO curves cross, leading to a \( K \)-factor.
Figure 9. The single jet inclusive distribution at $E_T = 100$ GeV, appropriate for Run I of the Tevatron. Theoretical predictions are shown at LO (dotted magenta), NLO (dashed blue) and NNLO (red). Since the full NNLO calculation is not complete, three plausible possibilities are shown.

(see below) near unity. A different strategy is to pick the scale at which the LO and NLO predictions coincide. By definition, the $K$-factor is unity with this scheme. In the case of inclusive jet production, one can see that these two scales are rather different – around 10 GeV and 200 GeV respectively. Finally, a rather different motivation comes from the consideration of a “physical” scale for the process. For instance, in the case of $W$ production, one might think that a natural scale is the $W$ mass. Clearly, these three typical methods for choosing the scale at which cross sections should be calculated do not in general agree. If they do, one may view it as a sign that the perturbative expansion is well-behaved. If they do not agree then the range of predictions provided by the different choices can be ascribed to the “theoretical error” on the calculation.

3.3. The NLO $K$-factor

The $K$-factor for a given process is a useful shorthand which encapsulates the strength of the NLO corrections to the lowest order cross section. It is calculated by simply taking the ratio of the NLO to the LO cross section. In principle, the $K$-factor may be very different for various kinematic regions of the same process. In practice, the $K$-factor often varies slowly and may be approximated as one number.

However, when referring to a given $K$-factor one must take care to consider the cross section predictions that entered its calculation. For instance, the ratio can depend quite strongly on the PDF’s that were used in both the LO and NLO evaluations. It is by now standard practice to use a NLO PDF (for instance, the CTEQ6M set) in evaluating the NLO cross section and a LO PDF (such as CTEQ6L) in the lowest order calculation. Sometimes this is not the case, instead the same PDF set may be used for
Table 1. $K$-factors for various processes at the Tevatron and the LHC, calculated using a selection of input parameters. In all cases, the CTEQ6M PDF set is used at NLO. $K$ uses the CTEQ6L1 set at leading order, whilst $K'$ uses the same set, CTEQ6M, as at NLO. Jets satisfy the requirements $p_T > 15$ GeV and $|\eta| < 2.5$ (5.0) at the Tevatron (LHC). In the $W + 2$ jet process the jets are separated by $\Delta R > 0.52$, whilst the weak boson fusion (WBF) calculations are performed for a Higgs of mass 120 GeV.

<table>
<thead>
<tr>
<th>Process</th>
<th>Typical scales</th>
<th>Tevatron K-factor</th>
<th>LHC K-factor</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\mu_0$</td>
<td>$\mu_1$</td>
<td>$K(\mu_0)$</td>
</tr>
<tr>
<td>$W$</td>
<td>$m_W$</td>
<td>$2m_W$</td>
<td>1.33</td>
</tr>
<tr>
<td>$W + 1$ jet</td>
<td>$m_W$</td>
<td>$\langle p_T^{\text{jet}} \rangle$</td>
<td>1.42</td>
</tr>
<tr>
<td>$W + 2$ jets</td>
<td>$m_W$</td>
<td>$\langle p_T^{\text{jet}} \rangle$</td>
<td>1.16</td>
</tr>
<tr>
<td>$t\bar{t}$</td>
<td>$m_t$</td>
<td>$2m_t$</td>
<td>1.08</td>
</tr>
<tr>
<td>$b\bar{b}$</td>
<td>$m_b$</td>
<td>$2m_b$</td>
<td>1.20</td>
</tr>
<tr>
<td>Higgs via WBF</td>
<td>$m_H$</td>
<td>$\langle p_T^{\text{jet}} \rangle$</td>
<td>1.07</td>
</tr>
</tbody>
</table>

both predictions. Of course, if one wants to estimate the NLO effects on a lowest order cross section, one should take care to match the appropriate $K$-factor.

A further complication is caused by the fact that the $K$-factor can depend quite strongly on the region of phase space that is being studied. The $K$-factor which is appropriate for the total cross section of a given process may be quite different from the one when stringent analysis cuts are applied. For processes in which basic cuts must be applied in order to obtain a finite cross section, the $K$-factor again depends upon the values of those cuts. Lastly, of course, as can be seen from Figure 9 the $K$-factor depends very strongly upon the renormalization and factorization scales at which it is evaluated. A $K$-factor can be less than, equal to, or greater than 1, depending on all of the factors described above.

As examples, in Table 1 we show the $K$-factors that have been obtained for a few interesting processes at the Tevatron and the LHC. In each case the value of the $K$-factor is compared at two often-used scale choices. For comparison, we also note the $K$-factor that is obtained when using the same (CTEQ6M) PDF set at leading order and at NLO. In general, the difference when using CTEQ6L1 and CTEQ6M at leading order is not great. However, for the case of bottom production, the combination of the large difference in $\alpha_s(m_b)$ and the gluon distribution at small $x$, result in very different $K$-factors. The values $K'$ may, for instance, be useful in performing a NLO normalization of parton shower predictions, as we shall discuss in later sections.

Such $K$-factors can be used as estimators for the NLO corrections for the listed processes in situations where only the leading order cross sections are available (for instance, when using a parton shower prediction). Note that, for the case of $W +$ jet production, we have two relevant scales for the hard scattering process: $m_W$ and the minimum allowed $p_T^{\text{jet}}$. If this threshold is quite low, as is the case in most studies at the Tevatron, these scales are quite different. Thus, there can be a fairly large variation
in the size of the predicted cross section even at NLO, as illustrated in Figure 10. In
the leading order calculation, the cross section varies by about a factor of 2.5 over the
range of scales shown. Although this variation is reduced considerably at NLO, the
cross section still increases by about 40% when moving from the highest scale shown to
the lowest.

4. NNLO

With all the advantages of NLO, it is only natural to consider going deeper into the
perturbative expansion. In the same sense that one only gains a reliable prediction
of an observable at NLO, the first meaningful estimate of the theoretical error comes
at NNLO. Further reduction of scale uncertainties is expected and, as we shall see, in
cases where NLO corrections are large, it is a chance to check the convergence of the
perturbative expansion.

With these sorts of justifications in mind, a recent goal of theoretical effort has
been the calculation of the 3 jet rate in $e^+e^-$ annihilation to NNLO. Together with data
from LEP and the SLC, this could be used to reduce the error on the measurement of
$\alpha_s(M_Z)$ to a couple of percent. However, the ingredients of a NNLO calculation are
both more numerous and more complicated than those entering at NLO. The different
contributions can best be understood by considering all possible cuts of a relevant
$O(\alpha_s^3)$ three-loop diagram, as shown in Figure 11.

The first contribution, represented by cut (a) in Figure 11, corresponds to 2-loop
3-parton diagrams. As the result of much innovative work over the last few years, this
contribution is now known (see, for example, references [4]–[6] of [33]). The contribution
labelled by (b) corresponds to the square of the 1-loop 3-parton matrix elements, the
same ones which appear (interfered with tree-level) in the NLO calculation [26, 30]. The third contribution (c) also contains 1-loop matrix elements, this time with 4 partons in the final state, one of which is unresolved. As in a NLO calculation, when one parton is unresolved this contribution diverges and a method must be developed to extract all singularities. Both these matrix elements [34, 35, 36, 38] and such methods (for instance, [39] and references therein) have been known for some time. The final contribution (d) involves only tree-level 5-parton matrix elements, but has so far proven the stumbling block to a complete NNLO 3-jet calculation. This piece contains two unresolved partons and, just as before, this gives rise singularities that must be subtracted. However, at present no general procedure for doing this exists and instead calculations can only be performed on a case-by-case basis. Quite recently a method has been developed for $e^+e^- \rightarrow$ jets calculations which has been used to calculate the doubly-unresolved sub-leading in $N_c$ contribution to the 3-jet rate [33]. Such progress bodes well for the completion both of this calculation and the closely related 2-jet rate at hadron colliders ‡.

The calculation that we have described represents the current frontier of NNLO predictions. For slightly simpler $2 \rightarrow 1$ and $2 \rightarrow 2$ processes, NNLO results are already available. The total inclusive cross section for the Drell-Yan process, production of a lepton pair by a $W$ or $Z$ in a hadronic collision, has long been known to NNLO accuracy [42]. In recent years the inclusive Higgs boson cross section, which is also a ‡ A consistent NNLO calculation at a hadron collider also requires parton densities evolved at the same order, which is now possible thanks to the calculation of the QCD 3-loop splitting functions [40, 41]. The differences between NLO and NNLO parton densities are reasonably small, though.
Figure 12. The inclusive Higgs cross section as a function of the Higgs boson mass.

The one-scale problem in the limit of large $m_t$, has also been computed at NNLO [43, 44]. For both these processes, the NLO corrections had already been observed to be large and the inclusion of the NNLO terms only provided a small further increase, thus stabilizing the perturbative expansion of these cross sections. This is illustrated in Figure 12, which shows the inclusive Higgs cross section at the LHC at each order of perturbation theory.

The above calculations have now been extended to include rapidity cuts on the leptons in the Drell-Yan process, in order to be more applicable for studies at the LHC [45]. These calculations extend the method used in [44], which uses an ingenious trick to bypass the problems associated with doubly-unresolved radiation that we have described above. In this approach, the phase space integrals are related to 2-loop integrals that are known and whose calculation can be automated. In this way, NNLO predictions can be provided for simple quantities such as rapidities. Further developments now allow for the introduction of generic cuts, paving the way for more detailed experimental analyses [46].

5. All orders approaches

Rather than systematically calculating to higher and higher orders in the perturbative expansion of a given observable, a number of different “all-orders” approaches are also commonly used to describe the phenomena observed at high-energy colliders. These alternative descriptions are typically most useful under a different set of conditions than a fixed order approach. The merging of such a description with fixed-order calculations, in order to offer the best of both worlds, is of course highly desirable.
Resummation is one such approach, in which the dominant contributions from each order in perturbation theory are singled out and “resummed” by the use of an evolution equation. Near the boundaries of phase space, fixed order predictions break down due to large logarithmic corrections, as we have seen above. A straightforward example is provided by the production of a vector boson at hadron colliders. In this case, two large logarithms can be generated. One is associated with the production of the vector boson close to threshold ($\hat{s} = Q^2$) and takes the form $\alpha_s^n \log^{2n-1} (1-z)/(1-z)$, where $z = Q^2/\hat{s} - 1$. The other logarithm, as illustrated earlier, is associated with the recoil of the vector boson at very small transverse momenta $Q_T$, so that logarithms appear as $\alpha_s^n \log^{2n-1} (Q^2/Q_T^2)$, c.f. Equation 5. Various methods for performing these resummations are available [need some refs], with some techniques including both effects at the same time [more refs]. As we shall see later, the inclusion of such effects is crucial in order to describe data at the Tevatron and to estimate genuine non-perturbative effects. Resummation is of course not restricted to the study of these processes alone, with much progress recently in the resummation of event shape variables at hadron colliders (for a recent review, see [47]).

The expression for the $W$ boson transverse momentum in which the leading logarithms have been resummed to all orders is given by (c.f. Equations 5 and 13),

$$\frac{d\sigma}{dp_T^2} = \sigma \frac{d}{dp_T^2} \exp \left( -\frac{\alpha_s C_F}{2\pi} \log^2 \frac{M_W^2}{p_T^2} \right).$$

(22)

This describes the basic shape for the transverse distribution for $W$ production, which is shown in Figure 13. Note that in this approximation the $p_T$ distribution vanishes as $p_T \to 0$, a feature which is not seen experimentally. However this can be explained by the fact that the only configuration included as $p_T \to 0$ is the one in which all emitted
gluons are soft. In reality (and in a more complete resummed prediction), multiple gluon emissions with a vector sum equal to $p_T$ contribute and fill in the dip at $p_T = 0$.

A different, but related, approach is provided by parton showers. The numerical implementation of a parton shower, for instance in the programs PYTHIA and HERWIG, is a common tool used in many current physics analyses. By the use of the parton showering process, a few partons produced in a hard interaction at a high energy scale can be related to partons at an energy scale close to $\Lambda_{QCD}$. At this lower energy scale, a universal non-perturbative model can then be used to provide the transition from partons to the hadrons that are observed experimentally. This is possible because the parton showering follows an evolution equation that can be solved either analytically or numerically. The solution of this evolution equation can be cast in the form of a Sudakov form factor, which indicates the probability of evolving from a higher scale to a lower scale without the emission of a gluon greater than a given value. For the case of parton showers from the initial state, the evolution proceeds backwards from the hard scale of the process to the cutoff scale, with the Sudakov form factors being weighted by the parton distribution functions at the relevant scales.

In the parton showering process, successive values of an evolution variable $t$, a momentum fraction $z$ and an azimuthal angle $\phi$ are generated, along with the flavors of the partons emitted during the showering. The evolution variable $t$ can be the virtuality of the parent parton (as in Pythia versions 6.2 and earlier), $E^2 (1-\cos \theta)$, where $E$ is the energy of the parent parton and $\theta$ is the opening angle between the two partons (as in Herwig), or the square of the relative transverse momentum of the two partons in the splitting (as in Pythia 6.3). The Herwig evolution variable has angular ordering built in, angular ordering is implicit in the Pythia 6.3 [48] evolution variable, and angular ordering has to be imposed after the fact for the Pythia 6.2 evolution variable. Angular ordering represents an attempt to simulate more precisely those higher order contributions that are enhanced due to soft gluon emission.

Note that with parton showering, we in principle introduce two new scales, one for initial state parton showering and one for the shower in the final state. In the Pythia Monte Carlo, the scale used is most often related to the maximum virtuality in the hard scattering, although a larger scale, such as the total centre-of-mass energy, can also be chosen. The Herwig showering scale is determined by the specific colour flow in the hard process and is related to the mass of the colour string.

We can write an expression for the Sudakov form factor of an initial state parton in the form shown in Equation 23, where $t$ is the hard scale, $t_o$ is the cutoff scale and $P(z)$ is the splitting function for the branching under consideration.

$$\Delta(t) \equiv \exp \left[ - \int_{t_0}^{t} \frac{dt'}{t'} \int \frac{dz}{z} \frac{\alpha_s}{2\pi} P(z) \frac{f(x/z, t')}{f(x, t)} \right]$$  \hspace{1cm} (23)

The Sudakov form factor has a similar form for the final state but without the PDF weighting. The introduction of the Sudakov form factor resums all the effects of soft and collinear gluon emission, which leads to well-defined predictions even in these regions. However, this ability comes at a price. Although the soft and collinear regions are
logarithmically enhanced and thus the dominant effect, this method omits the non-singular contributions that are typical of large energy, wide angle gluon emission. We shall return to this discussion later.

5.1. Sudakov form factors

As discussed in the previous section, the Sudakov form factor gives the probability for a parton to evolve from a harder scale to a softer scale without emitting a parton harder than some resolution scale, either in the initial state or in the final state. Sudakov form factors form the basis for both parton showering and resummation. Typically, the details of the form factors are buried inside the interior of such programs. It is useful, however, to generate plots of the initial state Sudakov form factors for the kinematic conditions encountered at both the Tevatron and LHC. Such plots indicate the likelihood for for the non-radiation of gluons from the initial state partons, and thus conversely for the radiation of at least one such gluon. Thus, they can also serve as a handy reference for the probability of jets from initial state radiation. A Sudakov form factor will depend on: (1) the parton type (quark or gluon), (2) the momentum fraction $x$ of the initial state parton, (3) the hard and cutoff scales for the process and (4) the resolution scale for the emission. Several examples are discussed below. These plots were generated with the Herwig++ parton shower formalism [49].

In Figure 14 are plotted the Sudakov form factors for the splitting $g \to gg$, at a hard scale of 100 GeV/c, and for several different values of the parton $x$ value. The form factors are plotted versus the resolution scale for the emitted gluon, which can be though of roughly as the transverse momentum of the emitted gluon. The probability for no emission decreases as the transverse momentum of the emitted gluon decreases and as the parton $x$ decreases. The former is fairly obvious; the latter may not be so.

**Figure 14.** The Sudakov form factors for initial state gluons at a hard scale of 100 GeV/c as a function of the transverse momentum of the emitted gluon. The form factors are for (top to bottom) parton $x$ values of 0.3,0.1,0.03,0.01,0.001 and 0.0001.
The smaller the value of the initial parton momentum fraction, the larger is the possible phase space for gluon emission.

For example, the probability for a gluon with an $x$ value of 0.03 to evolve from 100 GeV/c down to 10 GeV/c without emitting a gluon of 10 GeV/c or greater can be read off the plot as being 60%; thus the probability for at least one such emission is 40%. This is another example where the probability of emission of a hard gluon is enhanced by a logarithm (in this case the ratio of the hard scale to the resolution scale) compared to the naive expectation of a factor of $\alpha_s$. The probability of emission of such a gluon from an initial state gluon on the opposite side of the collision would of course be the same.

In Figure 15, the same Sudakov form factors are plotted but now using a hard scale of 500 GeV/c. The increased probability of a hard gluon emission can be observed. In Figures 16 and 17, the Sudakov form factors are plotted for the hard scales of 100 GeV/c and 500 GeV/c as before, but now for the splitting $q \to qg$. The probability of no emission is larger, due to the smaller color factor of the initial state quark compared to the gluon. Note that the form factor curves for $x$ values of less than 0.03 have not been plotted as they would essentially lie on top of the $x = 0.03$ curve. It is not the smaller color factor that causes the difference with the gluon but rather the splitting function. The splitting function for $g \to gg$ has singularities both as $z \to 0$ and as $z \to 1$, while the $q \to qg$ has only the $z \to 1$ singularity. Thus, for the $q \to qg$ splitting, there is not much to gain from decreasing $x$ on a logarithmic scale, as there is no singularity at $z = 0$ in the splitting function.
6. Partons and jet algorithms

In the detectors of experiments at the Tevatron and the LHC, collimated beams of particles are observed. In order to categorize these events, the hadrons are collected into jets using a jet algorithm. To make a comparison with a theoretical calculation of the types we have been discussing, it is necessary to also apply a jet algorithm at the parton level. Ideally, one would like an algorithm which yields similar results at the experimental (hadron) and theoretical (parton) levels. The goal is to characterize the short-distance physics event-by-event, in terms of the jets formed by the algorithm.

There are two essential stages for any jet algorithm. First, the objects belonging to
a cluster are identified. Second, the kinematic variables defining the jet are calculated from the objects defining the cluster. The two stages are independent. For the latter stage, using the jet algorithms developed for Run 2 at the Tevatron, the jet kinematic properties are defined (using a 4-vector recombination scheme) in terms of: $p_{\text{jet}}$, $p_T^{\text{jet}}$, $y^{\text{jet}}$ and $\phi^{\text{jet}}$.

At the experimental or simulated data level, jet algorithms cluster together objects such as particles or energies measured in calorimeter cells. At the theoretical level, partons are clustered. The goal of a jet algorithm is to produce similar results no matter the level it is applied. For a $2 \to 2$ LO calculation, a jet consists simply of 1 parton and no jet algorithm is necessary. As more partons are added to a calculation, the complexity of a jet grows and approaches the complexity found either in parton shower Monte Carlos or in data. For all situations in which a jet can consist of more than 1 parton, a completely specified jet algorithm is needed. The clustering algorithms rely on the association of these objects based on transverse momentum (the $k_T$ algorithm) or angles (the cone algorithm), relative to a jet axis.

For NLO calculations, as for example $W + 2$ jets, a jet can consist of either 1 or 2 partons. Cone jet algorithms as currently used by the Tevatron experiments require the use of seeds (initial directions for jet cones) as the starting points for jet searches. For a partonic level final state, the seeds are the partons themselves. The Run 2 cone algorithm (midpoint) places additional seeds between stable cones having a separation of less than twice the size of the clustering cones; the use of these additional seeds removes problems with infrared instabilities in theoretical calculations. Without a midpoint seed, a jet could be formed/not formed depending on the presence of a soft gluon between two hard partons; this leads to an undesirable logarithmic dependence of the cross section on the energy of this soft gluon.

With a cone algorithm, two partons are nominally included in the same jet if they are within $R_{\text{cone}}$ of the $p_T$-weighted jet centroid, and so within $\Delta R$ of 1.4 if a cone radius of 0.7 is used. However, it was noted that with the experimental jet algorithms used at the Tevatron, that two jets would not be merged into a single jet if they were separated by a distance greater than 1.3 times the cone radius. Thus, a phenomenological parameter $R_{\text{sep}} = 1.3$ was added to the theoretical prediction; two partons would not be merged into a single jet if they were separated by more than $R_{\text{sep}} \times R_{\text{cone}}$ from each other. So, in a parton level calculation having at most 3 partons in the final state, two partons are merged into the same jet if they are within $R_{\text{cone}}$ of the $p_T$-weighted jet centroid and within $R_{\text{sep}} \times R_{\text{cone}}$ of each other; otherwise the two partons are termed separate jets. Thus, for $W + 2$ jet production at NLO, the final state can consist of either 2 or 3 partons. The 2 parton final state will always be reconstructed as 2 jets; the 3 parton final state may be reconstructed as either 2 or 3 jets depending on whether the 2 lowest $p_T$ partons satisfy the clustering criteria described above. Note that for some partonic level programs such as JETRAD, the clustering is not performed prior to the evaluation of the matrix element. Thus, the individual transverse momenta of the jets are also not known at this time; only the transverse momentum of the highest $p_T$
parton, which by momentum conservation must remain unclustered, is known. For this reason, a renormalization/factorization scale of $p_T^{max}$ (the $p_T$ of this parton) is used in calculating the cross section for each jet.

A schematic diagram indicating the regions in which two partons will be included in the same jet is shown in Figure 18 [50]. All partons within $R_{cone}$ of each other will always be clustered in the same jet. This corresponds to the region labeled I. An ideal cone algorithm acting on data would cluster together only the underlying parton level configurations corresponding to region II and not configurations in region III. However, as will be seen in Section 5, the stochastic character of the parton showering + hadronization process makes such a clean division difficult in either real data or with a parton shower Monte Carlo. Because the matrix element for the emission of an additional real parton has both a collinear and soft pole, configurations in regions II and III with two partons having $\Delta R$ near 0.7 and $z$ near 0 will be most heavily populated.

The $k_T$ algorithm is conceptually simpler at all levels. Two partons (or particles, or energies) in calorimeter towers are combined if their relative transverse momentum is less than a given measure. At the parton level, each parton is considered as a proto-jet. The quantities $k_{T,i}^2 = P_{T,i}^2$ and $k_{T,(i,j)} = \min(P_{T,i}^2, P_{T,j}^2) \Delta R_{i,j}^2 / D^2$ are computed for each parton and each pair of partons respectively. $P_{T,i}$ is the transverse momentum of the $i^{th}$ parton, $\Delta R_{i,j}$ is the distance (in $y, \phi$ space) between each pair of partons, and $D$ is a parameter that controls the size of the jet. If the smallest of the above quantities is a $k_{T,i}$ then that parton becomes a jet; if the smallest quantity is a $k_{T,(i,j)}$, then the two partons are combined into a single protojet by summing their four-vector components. In a NLO inclusive jet calculation, the two lowest $p_T$ partons may be combined into a single jet, and thus the final state can consist of either 2 or 3 jets, as was also true for the case of the cone algorithm.

The assumption we are making above is that the jets of hadrons measured in a collider experiment can be represented by the 1 or 2 partons that comprise a jet at
the NLO theoretical level. That is, the 1 or 2 partons present in a NLO jet effectively represent the many partons produced by a parton shower. For example, an equivalent description of the jet shape is provided by the two types of calculation.

This approximation has been borne out in practice with one remaining correction being necessary. Partons whose trajectories lie inside the jet cone eventually produce hadrons, some of which may land outside the cone due to the fragmentation process. The fragmentation correction takes a particularly simple form. For a cone of radius 0.7, each jet loses approximately 1 GeV due to fragmentation, basically independent of the jet transverse energy. The naïve assumption might be that the energy outside the cone due to fragmentation would rise with the jet energy; however, the jet becomes narrower at higher $E_T$, leading to a roughly constant amount of energy in the outermost portions of the jet. As will be described in Section 5, corrections also need to be applied to the data or to the theory to take into account the underlying event energy.

7. Merging parton showers and fixed order

As we have discussed previously, parton showers provide an excellent description in regions which are dominated by soft and collinear gluon emission. On the other hand, matrix element calculations provide a good description of processes where the partons are energetic and widely separated and, in addition, include the effects of interference between amplitudes with the same external partons. But, on the other hand, the matrix element calculations do not take into account the interference effects in soft and collinear gluon emissions which cannot be resolved, and which lead to a Sudakov suppression of such emissions.

Clearly, a description of a hard interaction which combines the two types of calculations would be preferable. For this combination to take place, there first needs to be a universal formalism that allows the matrix element calculation to “talk” to the parton shower Monte Carlo. Such a universal formalism was crafted during the Les Houches Workshop on Collider Physics in 2001 and the resulting “Les Houches Accord” is in common use [51]. The accord specifies an interface between the matrix element and the parton shower program which provides information on the the parton 4-vectors, the mother-daughter relationships, and the spin/helicities and color flow. It also points to intermediate particles whose mass should be preserved in the parton showering. All of the details are invisible to the casual user and are intended for the matrix element/parton shower authors.

Some care must be taken however, as a straight addition of the two techniques would lead to double-counting in kinematic regions where the two calculations overlap. There have been many examples where matrix element information has been used to correct the first or the hardest emission in a parton shower. There are also more general techniques that allow matrix element calculations and parton showers to each be used in kinematic regions where they provide the best description of the event properties and that avoid double-counting. One such technique is termed CKKW [52].
With the CKKW technique, the matrix element description is used to describe parton branchings at large angle and/or energy, while the parton shower description is used for the smaller angle, lower energy emissions. The phase space for parton emission is thus divided into two regions, matrix element dominated and parton shower dominated, using a resolution parameter \( d_{\text{ini}} \). The argument of \( \alpha_s \) at all of the vertices is chosen to be equal to the resolution parameter \( d_i \) at which the branching has taken place and Sudakov form factors are inserted on all of the quark and gluon lines to represent the lack of any emissions with a scale larger than \( d_{\text{ini}} \) between vertices. The \( d_i \) represent a virtuality or energy scale. Parton showering is used to produce additional emissions at scales less than \( d_{\text{ini}} \). A schematic representation of the CKKW scheme is shown in Figure 19 for the case of \( W^+ \) jets production at a hadron-hadron collider. A description of a \( W + 2 \) jet event in the NLO formalism is also shown for comparison.

The CKKW procedure provides a matching between the matrix element and parton shower that should be correct to the next-to-leading-logarithm (NLL) level. There are, however, a number of choices that must be made in the matching procedure that do not formally affect the logarithmic behavior but do affect the numerical predictions, on the order of 20-30%. The CKKW procedure gives the right amount of radiation but tends to put some of it in the wrong place with the wrong color flow. Variations that result from these choices must be considered as part of the systematic error inherent in the CKKW process. This will be discussed further in Section 5.

For the CKKW formalism to work, matrix element information must in principle be available for any number \( n \) of partons in the final state. Practically speaking, having information available for \( n \) up to 4 is sufficient for the description of most events at the Tevatron or LHC. The CKKW formalism is implemented in the parton shower Monte Carlo SHERPA [53] and has also been used for event generation at the Tevatron and LHC using the Mrenna-Richardson formalism [54]. An approximate version of CKKW matching (the mlm approach §) is available in ALPGEN 2.0 [3].

8. Merging NLO calculations and parton showers

A combination of NLO calculations with parton shower Monte Carlos leads to the best of both worlds. The NLO aspect leads to a correct prediction for the rate of the process and also improves the description of the first hard parton emission. The parton shower aspect provides a sensible description of multiple/soft collinear emissions with a final state consisting of hadrons, which can then be input to a detector simulation. In a parton shower interface, a specific subtraction scheme must be implemented to preserve the NLO cross section. As each parton shower Monte Carlo may produce a different real radiation component, the subtraction scheme must necessarily depend on the Monte Carlo program to which the matrix element program is matched. The presence of interference effects with NLO calculations requires that a relatively small fraction (\( \sim 10\% \)) of events have negative weights (of value \(-1\)).

§ ...which one of the authors takes credit for naming.
Several groups have worked on the subject to consistently combine partonic NLO calculations with parton showers.

- Collins, Zu [55, 56]
- Frixione, Nason, Webber (MC@NLO) [57, 58, 59]
- Kurihara, Fujimoto, Ishikawa, Kato, Kawabata, Munchisa, Tanaka [60]
- Krämer, Soper [61, 62, 63]
- Nagy, Soper [64, 65]

MC@NLO is the only publically available program that combines NLO calculations with parton showering and hadronization. The Herwig Monte Carlo is used for the latter. The use of a different Monte Carlo, such as Pythia, would require a different subtraction scheme for the NLO matrix elements. The processes included to date are: ($W, Z, \gamma *, H, b\bar{b}, t\bar{t}, HW, HZ, WW, WZ, ZZ$). Recently, single top hadroproduction has been added to MC@NLO [66]. This is the first implementation of a process that has both initial- and final-state singularities. This allows a more general category of additional processes to be added in the future. Work is proceeding on inclusion of inclusive jet production and WW fusion to Higgs. Adding spin correlations to a process increases the level of difficulty but is important for processes such as single top production.

If, in addition, the CKKW formalism could be used for the description of hard parton emissions, the utility and accuracy of a NLO Monte Carlo could be greatly
increased. The merger of these two techniques should be possible in Monte Carlos available by the time of the LHC turn-on.

9. Acknowledgements

10. References

[9] H. Murayama, I. Watanabe and K. Hagiwara, KEK-91-11