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Interpolation von QCD Wirkungsquerschnitten unter Verwendung von APPLGRID und fastNLO

Interpolation of QCD cross sections using
APPLGRID and fastNLO

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Abstract

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The interpolation methods implemented by `APPLGRID` and `fastNLO` are validated for a NLO calculation of inclusive Higgs boson production at the 13 TeV LHC. Different final state jet multiplicities are studied. It is verified that the method accurately reproduces observables with *a posteriori* parameter variation. The `MCgrid` software is used to interface the interpolation tools and automatically produce interpolation grids for fixed order NLO calculations.

Key words: perturbative QCD; NLO QCD calculations; Monte Carlo event generator; PDF

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1 Introduction

Run 1 of the Large Hadron Collider (LHC) displayed great performance of the collider and its detectors. It enabled high precision tests of theoretical predictions at unprecedented center of mass energies. Simultaneously it encouraged theorists to expend huge effort in minimizing the uncertainties of calculations in quantum chromodynamics. A great amount of progress could be achieved, among others the automation of next-to-leading order (NLO) calculations, the merging of parton shower results with different jet multiplicities and the matching of parton showers to NLO-accuracy calculations [1]. As of 3 June this year, the LHC is delivering data again at an even higher center of mass energy of 13 TeV. The new run promises new results and an increase in statistics, allowing for a more detailed study of many observations.

Precise predicting of the expected results is crucial in a test of our current models. To achieve this, uncertainties in the calculations have to be as small as possible. However, with rising complexity the calculations become lengthy. Single computations lasting for days are not uncommon even at NLO. This is aggravated by the fact that they have to be repeated with different values of the coupling parameter α_s , at different scales and with different parton distribution functions (PDFs) in order to get a reasonable estimate of the uncertainty. Including PDF uncertainties is especially expensive as it involves a large number of repeated calculations. PDF fitting groups, who include many different processes in their fits to the data, suffer

from this particularly. Without any speedup, their task would be impossible. For this reason, methods have been developed to accelerate the process of varying the parameters, obviating the need for explicit recalculations. One method is based on a special event file format, that stores all information required to recompute NLO observables with different parameters [2]. A different approach is the on-the-fly reweighting that has been introduced in the 2.2.0 release of the Monte Carlo event generator **SHERPA** [3]. The fastest currently possible reevaluations are achieved with interpolation tools like **APPLGRID** [4] and **fastNLO** [5]. Two interfaces exist that allow the automated creation of the related interpolation grids in NLO calculations, namely **aMCfast** [6] and **MCgrid** [7].

Currently, **MCgrid** supports calculations at LO, NLO and the fixed-order expansion of **MC@NLO**. One of the goals of the project is the support of multijet merging calculations. Along this road, it has to be validated that the interpolation method works correctly when the different jet multiplicities are treated separately. In this thesis, the process of Higgs boson production through gluon fusion in combination with different jet multiplicities is considered. It had not been verified yet, that it is supported by **MCgrid**. After the discovery of the Higgs boson [8, 9], one of the tasks of the 13 TeV LHC will be the determination of its properties. Increased statistics will allow the study of differential cross sections for the first time. It is therefore important to enable the detailed analysis of theoretical uncertainties in this process.

This thesis is organized as follows. First, in chapters 2 and 3, an overview of the theoretical foundations involved in the calculations is given. It is followed by an illustration of the gluon fusion process in chapter 4. There, a brief study of the Higgs transverse momentum in perturbative QCD is included. In chapter 5 the interpolation method implemented by **MCgrid** is validated for the gluon fusion process with different jet multiplicities. Proof is provided that it is possible to vary the QCD parameters *a posteriori* using either **APPLGRID** or **fastNLO**. Two application examples are presented in chapter 6. They are supposed to demonstrate the usefulness of the method. The thesis finishes with a conclusion and an outlook on possible extensions in the future.

2 Basics of perturbative QCD

The following sections give an overview of the basic principles that provide the basis for perturbative QCD. They include the most important aspects regarding numerical calculations. It is by far no complete depiction but it covers the parts that play a key role in the calculations used for this thesis.

2.1 The QCD Lagrangian

QCD is the quantum field theory that describes the strong interactions between quarks and gluons. Mathematically, it is a non-abelian gauge theory with symmetry group SU(3). Its Lagrangian is given by

$$\mathcal{L}_{\text{QCD}} = \sum_q \bar{\psi}_{q,a} (i\gamma^\mu \partial_\mu \delta_{ab} - g_s \gamma^\mu t_{ab}^C \mathcal{A}_\mu^C - m_q \delta_{ab}) \psi_{q,b} - \frac{1}{4} F_{\mu\nu}^A F^{A\mu\nu}, \quad (2.1)$$

where the sum goes over all quark flavors. The $\psi_{q,a}$ are quark-field spinors, where $a = 1 \dots 3$ denotes the color index, and the \mathcal{A}_μ^C are gluon fields with a color index $C = 1 \dots 8$. The strong coupling constant is denoted by g_s . Quarks transform under the fundamental representation of SU(3) while gluons transform under the adjoint representation. The t_{ab}^C are the generators of the group. The gluon field tensor $F_{\mu\nu}^A$ is given by

$$F_{\mu\nu}^A = \partial_\mu \mathcal{A}_\nu^A - \partial_\nu \mathcal{A}_\mu^A - g_s f_{ABC} \mathcal{A}_\mu^B \mathcal{A}_\nu^C, \quad (2.2)$$

where the f_{ABC} are the structure constants of the group, defined through $[t^A, t^B] = if_{ABC}t^C$. In comparison to quantum electrodynamics (QED), the main difference is the presence of the interaction term $-g_s f_{ABC} \mathcal{A}_\mu^B \mathcal{A}_\nu^C$ which results in the existence of 3-gluon and 4-gluon vertices.

The perturbative approach to QCD is to write the observables as a power series in $\alpha_s = g_s^2/(4\pi)$:

$$F = F^{(1)}\alpha_s + F^{(2)}\alpha_s^2 + \dots , \quad (2.3)$$

where $\alpha_s \ll 1$ so that the series can be truncated after a few terms to obtain a useful approximation. This leads to leading order (LO), next-to-leading order (NLO), next-to-next-to-leading order (NNLO)... predictions. A straightforward way to determine the coefficients is the use of Feynman Diagrams.

2.2 Renormalization and the running coupling

Calculations in perturbative QCD involve UV-divergent integrals. Luckily QCD is a renormalizable theory and therefore the divergences can be handled by regularization and renormalization. As a consequence, the quantities appearing in the Lagrangian (the “bare” quantities) are not the same as the quantities that are physically observed. In the renormalization process, an additional scale dependence is introduced which vanishes if we consider the whole perturbative series. The evolution of quantities with the renormalization scale μ_R is described by differential equations known as *renormalization group equations*. As an example, the “running” of the coupling constant is described by

$$\frac{d\alpha_s(\mu_R^2)}{d\ln \mu_R^2} = \beta(\alpha_s(\mu_R^2)) = -\alpha_s^2(b_0 + b_1\alpha_s + b_2\alpha_s^2 + \dots). \quad (2.4)$$

The minus sign in eq. (2.4) is responsible for the asymptotic freedom of QCD: As the momentum transfer becomes large, the strong coupling becomes weak so that quarks and gluons nearly behave as if they were free particles.

In leading order the analytic solution of eq. (2.4) is given by

$$\alpha_s(\mu_R^2) = \frac{\alpha_s(\mu_0^2)}{1 + b_0 \alpha_s(\mu_0^2) \ln \frac{\mu_R^2}{\mu_0^2}} \quad \text{with} \quad b_0 = \frac{11N_C - 2n_f}{12\pi}, \quad (2.5)$$

where N_C is the number of colors and n_f denotes the number of active flavors. This relates the coupling constant at a scale μ_R to the one at a reference scale μ_0 , where its value is known.

2.3 From parton model to QCD

The parton model was introduced in 1969 by Richard P. Feynman to describe high-energy particle collisions involving hadrons [10]. The basic assumption of the parton model is that all hadrons consist of point-like spin- $\frac{1}{2}$ particles (partons) which are responsible for their behavior in interactions. Furthermore, it is assumed that the hadron is in a reference frame where it carries infinite (or at least very high) momentum. In this infinite momentum frame the hadron suffers both Lorentz contraction and time dilation so that the distribution of partons within it does not change during the (vanishingly small) time of interaction. Thus each parton carries a definite fractional momentum x , with $0 < x < 1$. In addition, the process of hadronization due to quark confinement happens too late to influence the interaction. Another important consequence is that the probability of a parton influencing the scattering of another parton is suppressed (“incoherence” of the parton model). The reason this model works is the asymptotic freedom of the underlying theory. However, this also limits the applicability of the parton model to high energy cross sections.

By itself, the parton model does not make any assumptions about the distribution of partons inside the hadron. It just introduces it as a parameter in the form of *parton distribution functions* (PDFs) $f_i(x)$, which represent the probability of finding a parton of type i carrying a momentum fraction x of the hadron. As they cannot be derived from first principles they have to be extracted from measured data. This is the task of different PDF fitting groups like HERAPDF [11], CTEQ [12], MSTW [13] and NNPDF [14]. Parton model predictions then take the form of a convolution of the parton level interaction with the PDF, summarized over all possible parton

flavors. We call this the “naive” parton model.

The naive parton model works well as long as the energy scale is not too high. Otherwise we need to include higher order corrections which can arise from real emissions and virtual loops. These involve infrared divergences that cancel each other exactly thanks to the Kinoshita–Lee–Nauenberg theorem [15, 16], rendering perturbative QCD as a whole an infrared safe theory. However, the cancellation is not guaranteed if we truncate the perturbative series after a finite number of terms. In processes involving initial-state hadrons, the partons can emit gluons before entering the hard interaction (see fig. 2.1). However, there is an important difference between real and virtual emissions in this case: While the virtual emission does not change the momentum of the parton entering the process, the real gluon carries off parts of the parton momentum. Thus, the total cross section consists of two different hard cross sections that do not cancel in the collinear limit. This is a consequence of the collinear limit corresponding to long-range effects of the strong interaction, which are not calculable in perturbation theory.

In order to be able to calculate cross sections with initial-state hadrons, we can take a similar approach as for the renormalization of the coupling constant and introduce a scale variable which we call the *factorization scale* μ_F . All the non-perturbative parts are cut off at μ_F and absorbed into the PDF. There is an arbitrariness in how much of the correction terms is to be factored out. This is defined by the *factorization scheme*. Common schemes include the DIS scheme, in which all non-leading order contributions are absorbed into the PDFs, and the \overline{MS} scheme, in which only the divergent parts are absorbed. Once the factorization scheme has been chosen, it has to be used consistently in all following cross section calculations.

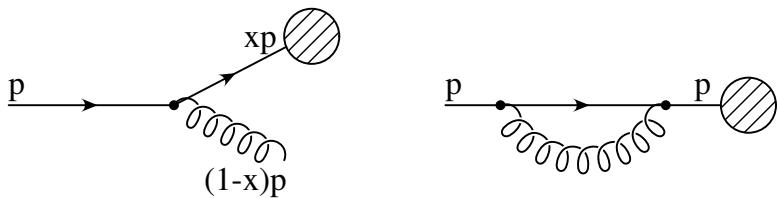


Figure 2.1: Feynman diagrams for initial-state gluon emission.

As an example, let us consider the cross section for a scattering process involving two initial state hadrons h and h' with momenta p and p' , which now takes the factorized form

$$\sigma_{h,h'} = \sum_{i,j} \int dx dx' f_{i/h}(x, \mu^2) \cdot \sigma_{ij}(xp, x'p', \alpha_s(\mu^2)) \cdot f_{j/h'}(x', \mu^2), \quad (2.6)$$

where we have taken $\mu_R = \mu_F = \mu$ and where the sum includes all possible initial state parton combinations. σ_{ij} denotes the hard parton-level cross section which can be calculated in perturbation theory. All the non-perturbative long-distance contributions are factorized into the PDFs.

2.4 DGLAP evolution

Analogous to the running coupling, we can define a renormalization group equation that describes the evolution of the PDFs with the factorization scale. It is called the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) equation [17–19] and takes the form of a matrix equation spanning all quark flavors and the gluon:

$$\begin{aligned} \frac{d}{d \ln \mu_F^2} \begin{pmatrix} q_i(x, \mu_F^2) \\ g(x, \mu_F^2) \end{pmatrix} &= \frac{\alpha_s(\mu_F^2)}{2\pi} \sum_{q_j, \bar{q}_j} \int_x^1 \frac{dz}{z} \\ &\cdot \begin{pmatrix} P_{q_i q_j}(\frac{x}{z}, \alpha_s(\mu_F^2)) & P_{q_i g}(\frac{x}{z}, \alpha_s(\mu_F^2)) \\ P_{g q_j}(\frac{x}{z}, \alpha_s(\mu_F^2)) & P_{gg}(\frac{x}{z}, \alpha_s(\mu_F^2)) \end{pmatrix} \begin{pmatrix} q_j(z, \mu_F^2) \\ g(z, \mu_F^2) \end{pmatrix}. \end{aligned} \quad (2.7)$$

The $P_{ij}(x, \alpha_s)$ are called splitting functions and they imply the probability of a parton splitting into two other partons. They are calculable in perturbation theory and are known up to NNLO [20, 21]. The DGLAP equation allows to evolve the PDFs from an initial scale Q_0 to another scale Q without further knowledge and thus is one of the most important equations of perturbative QCD.

2.5 Next-to-leading order calculations

When going from LO calculations at tree level to NLO, one has to take into account real emissions from the colored particles and virtual loops. In general, both the

real and the virtual corrections are separately divergent and need to be regularized. There are two general methods that are commonly used to take care of the infrared divergences in NLO calculations, namely the *slicing method* and the *subtraction method*. The slicing method introduces a small parameter δ , which slices the integration region into two pieces so that it can be computed numerically. A residual dependency on δ remains, which should be neglectable if δ is small. However, this has to be checked in an actual calculation. The advantage of the subtraction method is that it does not involve any approximations.

We can demonstrate the subtraction method with a simple example, that has been adopted from [22]. Consider the expression for the expectation value of an infrared-safe observable O at NLO accuracy, consisting of a Born (B), a virtual (V) and a real (R) term:

$$\langle O \rangle = \lim_{\epsilon \rightarrow 0} \int_0^1 dx x^{-2\epsilon} O(x) \left[\left(\frac{d\sigma}{dx} \right)_B + \left(\frac{d\sigma}{dx} \right)_V + \left(\frac{d\sigma}{dx} \right)_R \right]. \quad (2.8)$$

We assume that the cross sections can be written as

$$\left(\frac{d\sigma}{dx} \right)_B = B\delta(x), \quad (2.9)$$

$$\left(\frac{d\sigma}{dx} \right)_V = a \left(\frac{B}{2\epsilon} + V \right) \delta(x), \quad (2.10)$$

$$\left(\frac{d\sigma}{dx} \right)_R = a \frac{R(x)}{x}, \quad (2.11)$$

where B and V are constant factors and $\lim_{x \rightarrow 0} R(x) = B$. a denotes the coupling constant. Obviously, both the real and the virtual part are divergent in the limit

$\epsilon \rightarrow 0$. Using the subtraction method, we can rewrite the real contribution to obtain

$$\begin{aligned} \langle O \rangle_R &= a \lim_{\epsilon \rightarrow 0} \int_0^1 \frac{dx}{x^{1+2\epsilon}} O(x) R(x) \\ &= a BO(0) \lim_{\epsilon \rightarrow 0} \int_0^1 \frac{dx}{x^{1+2\epsilon}} + a \int_0^1 \frac{dx}{x} [O(x) R(x) - BO(0)] \\ &= -a BO(0) \lim_{\epsilon \rightarrow 0} \frac{1}{2\epsilon} + a \int_0^1 \frac{dx}{x} [O(x) R(x) - BO(0)]. \end{aligned} \quad (2.12)$$

By explicitly writing down the virtual part,

$$\langle o \rangle_V = a \lim_{\epsilon \rightarrow 0} \int_0^1 \frac{dx}{x^{2\epsilon}} O(x) \left(\frac{B}{2\epsilon} + V \right) \delta(x), \quad (2.13)$$

we see that the first term gets exactly canceled by the first term on the right hand side of eq. (2.12). Including the Born contribution we arrive at the expression

$$\langle O \rangle = BO(0) + a \left\{ VO(0) + \int_0^1 \frac{dx}{x} [O(x) R(x) - BO(0)] \right\}, \quad (2.14)$$

which now only consists of finite terms. The remaining integral can be evaluated using Monte Carlo methods. The subtraction method can be generalized to arbitrary hadronic cross sections, provided that the definition of the observables allows the cancellation of the divergences.

2.6 Parton showers

There are phase space regions that cannot be well described by fixed order calculations in perturbation theory. These include collinear parton splitting and soft gluon emission, which are closely related to the presence of infrared divergences. To describe them accurately, higher order terms need to be considered. However, the work required to derive the needed matrix elements quickly increases with each order, which is the reason why most processes have not been calculated further than NLO. We need a different approach to deal with the problematic phase space regions. Instead of relying on a fixed order calculation, we can consider an approximate model

that includes the dominant contributions at all orders. In this model, the collinear splitting and soft gluon emission of every parton in the initial and final state is simulated with respect to the related probabilities. The additional partons are again able to split or radiate gluons. By recursively applying this procedure, we obtain a cascade of parton emissions, called a *parton shower*. An example is illustrated in fig. 2.2. The shower ends when a certain cut-off scale is reached.

The evolution of the splitting with the decreasing scale is given by the DGLAP equation eq. (2.7). In this context the PDFs do not describe the momentum distributions of the partons inside of a hadron, but rather the distribution of the momentum fractions of the partons resulting from the splitting.

The computation of parton showers can be formulated in a way that is well suited for a Monte Carlo program. We can combine the parton shower program with a hadronization model, that combines both the initial state and the final state partons into colorless hadrons, beginning at the cutoff scale of the shower. We call the result a *parton shower Monte Carlo event generator*. It is a powerful tool that is able to

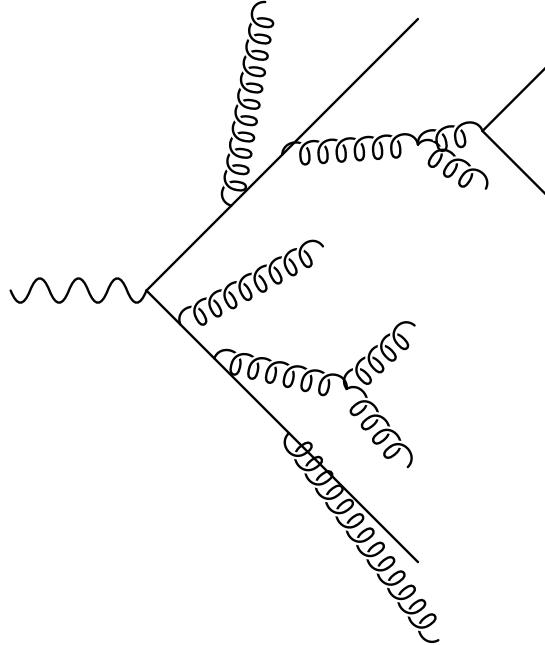


Figure 2.2: Example of a parton shower.

fully simulate QCD events in hadron collisions.

The main disadvantage of parton shower generators is that they are not guaranteed to properly describe events that include hard and large-angle emissions. Those events are, however, correctly described by fixed order calculations. To combine the benefits of both, algorithms have been developed that merge LO matrix elements and parton showers with different multiplicities (MEPS). The main issue in the course of this is double counting. An event with n partons in the final state can either be the product of an n -parton matrix element that has been showered with only soft and collinear emissions or it could be the product of an $(n - 1)$ -parton matrix element for which the showering led to the emission of a hard, large-angle gluon. Those cases have to be carefully separated to avoid an overrepresentation of the related phase space region. The most widely used methods to avoid double counting are CKKW matching [23, 24] and MLM matching [25, 26].

Another problem of parton shower predictions is that they suffer from strong scale dependence because they are based on LO matrix elements. Promoting parton showers to NLO accuracy is a much harder task because of divergent event weights. Nonetheless, there are methods to circumvent this problem and the two widely used solutions are **MC@NLO** [22] and **POWHEG** [27–29]. As of recently, it is also possible to merge different jet multiplicities in NLO calculations matched to parton showers [30–34].

3 Variation of QCD input parameters

Calculations in perturbative QCD comprise uncertainties which should be determined as good as possible when they are meant to be used for predictions. One source of uncertainty is the truncation of the perturbative series at some fixed order. The corrections due to higher terms can only be known exactly if those terms are evaluated explicitly. As that is no suitable approach, a good practice has evolved that consists of varying the renormalization and factorization scales in a specific range and checking how much the cross section changes by this variation. This is based on the fact that the scale parameters are arbitrary variables, introduced in the renormalization procedure, and have no physical meaning. Physical observables do not depend on the scale parameters and therefore in perturbative calculations a strong dependence on the scales indicates that higher order terms could give large corrections. Additional uncertainties come from the strong coupling constant α_s and the choice of the PDF. They suffer from errors in the experimental data and depend on the assumptions that are used during the fit.

For a differentiated estimate of the full uncertainty, a cross section calculation has to be repeated with different input values. When the number of variations becomes large, it is not practical to rerun the whole event generation for each calculation as the time and resource consumption become too high. Instead it is possible to reuse information from previously generated events and combine them with the new parameters. In the following, two different methods are presented.

3.1 Reweighting QCD calculations

If we want to change the parameters in a calculation, we need to know exactly, how the individual terms depend on those parameters. Here we consider an NLO calculation using Catani-Seymour subtraction [35], which is the scheme implemented in **SHERPA** and **MCgrid**. Other subtraction schemes can be used as well, as is demonstrated in [6] for the FKS scheme [36, 37].

The total cross section can be separated into four finite terms:

$$\sigma_{pp \rightarrow X}^{\text{NLO}} = \int d\hat{\sigma}^B + \int d\hat{\sigma}^V + \int d\hat{\sigma}^I + \int d\hat{\sigma}^{RS} \quad (3.1)$$

They correspond to the Born (B), virtual (V), integrated subtraction (I) and real subtraction (RS) parts of the calculation. We need to work out the explicit dependence on the parameters to accurately reweight them. For the B and RS terms this is straightforward as they resemble LO calculations. Making use of the factorization theorem we can write them in the form (cf. eq. (2.6))

$$\sigma^{B/RS} = \sum_{i,j} \int dx_1 dx_2 \int d\Phi_n \left(\frac{\alpha_s(\mu_R^2)}{2\pi} \right)^p f_i(x_1, \mu_F^2) f_j(x_2, \mu_F^2) d\hat{\sigma}, \quad (3.2)$$

where for the B term $p = p_{\text{LO}}$ and for the RS term $p = p_{\text{LO}} + 1$. Using Monte Carlo integration, we can rewrite this as a sum over generated events:

$$\int d\hat{\sigma}^{B/RS} = \sum_{e=1}^{N_{\text{evt}}} \alpha_s^p(\mu_R^2) f_1(x_1, \mu_F^2) f_2(x_2, \mu_F^2) w_e^{(0)}, \quad (3.3)$$

where the weight $w_e^{(0)}$ contains the parton-level matrix element squared.

The virtual part occupies a more complicated structure because the weights explicitly depend on the renormalization scale. It takes the form

$$\int d\hat{\sigma}^V = \sum_{e=1}^{N_{\text{evt}}} \alpha_s^{p_{\text{LO}}+1}(\mu_R^2) f_1(x_1, \mu_F^2) f_2(x_2, \mu_F^2) \left\{ w_e^{(0)} + l_R w_e^{(1)} + l_R^2 w_e^{(2)} \right\}, \quad (3.4)$$

with renormalization scale logarithms $l_R = \log\left(\frac{\mu_r^2}{\mu_{R,0}^2}\right)$, where $\mu_{R,0}$ is the scale at which $w_e^{(1)}$ and $w_e^{(2)}$ were originally evaluated.

In the I part, the event weights have a complex dependence on the PDF. The full structure can be written as

$$\int d\hat{\sigma}^I = \sum_{e=1}^{N_{\text{evt}}} \alpha_s^{p_{\text{LO}}+1}(\mu_R^2) \left\{ f_1(i, x_1, \mu_F^2) w_e^{(0)} f_2(j, x_2, \mu_F^2) \right. \\ + \left(\sum_{k=1}^4 f_1^{(k)}(i, x_1, x'_1, \mu_F^2) w_{e,k}^{(3)} \right) f_2(j, x_2, \mu_F^2) \\ \left. + f_1(j, x_1, \mu_F^2) \left(\sum_{k=1}^4 w_{e,k}^{(4)} f_2^{(k)}(j, x_2, x'_2, \mu_F^2) \right) \right\}, \quad (3.5)$$

where the x and x' are the Björken- x before and after initial state branching. Moreover, i and j denote the parton flavors before the branching and the $f^{(k)}$ provide the correct form of the PDF depending on the type of branching. They are given explicitly in [7].

We can dispose of the weights $w^{(1)}$ and $w^{(2)}$ by choosing a central scale. If we furthermore project the contributions from $w^{(3)}$ and $w^{(4)}$ onto separate events, we can write the total NLO cross section in the compact form

$$\sigma_{pp \rightarrow X}^{\text{NLO}} = \sum_{e=1}^{N_{\text{evt}}} \alpha_s^{p_e}(\mu_R^2) f_1(x_1, \mu_F^2) f_2(x_2, \mu_F^2) w_e, \quad (3.6)$$

Provided that all event weights have been stored, it is now possible to change the values of α_s , μ_R and μ_F or use a different PDF *a posteriori*.

3.2 Interpolation grids

Despite the advantage towards regenerating all events for the variation of a single parameter, the reweighting approach is still not a satisfying solution for many use cases. The whole event record has to be stored, which can easily reach many gigabytes or even terabytes in high statistics computations. The storing and reprocessing of the events may be a challenge by itself and is not convenient if more than a few parameter

variations have to be performed. One therefore wishes to somehow decrease the resource requirements without losing a significant amount of accuracy. In the ideal case, it should be mostly independent of the statistics. A possible solution is the use of interpolating grids to represent the PDFs and event weights. Then only a uniquely defined number of values has to be saved, while values in-between the grid points are generated by interpolating functions. Such a method has been implemented by the **APPLGRID** [4] and **fastNLO** [5, 38] projects.

The PDF $f(x, Q^2)$ depends on the momentum fraction x and the scale Q^2 . It can be approximated as a sum over discrete grid points using interpolation functions I of order N :

$$f(x, Q^2) = \sum_{i=0}^{N_x} \sum_{j=0}^{N_Q} f(x_i, Q_j^2) I_i^{(N_x)}(x_1) I_j^{(N_Q)}(Q^2). \quad (3.7)$$

Consequently, we can write eq. (3.6) as

$$\begin{aligned} \sigma_{pp \rightarrow X}^{\text{NLO}} &= \sum_{e=1}^{N_{\text{evt}}} \sum_{i,j=0}^{N_x} \sum_{k=0}^{N_Q} \alpha_s^{p_e}(Q_k^2) f_1(x_i, Q_k^2) f_2(x_j, Q_k^2) w_e \\ &\quad \cdot I_i^{(N_x)}(x_1) I_j^{(N_x)}(x_2) I_k^{(N_Q)}(Q^2) \\ &= \sum_p \sum_{i,j=0}^{N_x} \sum_{k=0}^{N_Q} \alpha_s^p(Q_k^2) f_1(x_i, Q_k^2) f_2(x_j, Q_k^2) W_{i,j,k}^{(p)}, \end{aligned} \quad (3.8)$$

where p is the perturbative order and the interpolated weights $W_{i,j,k}^{(p)}$ are processed as a sum over the events:

$$W_{i,j,k}^{(p)} = \sum_{e=1}^{N_{\text{evt}}} \delta_{p,p_e} w_e I_i^{(N_x)}(x_1) I_j^{(N_x)}(x_2) I_k^{(N_Q)}(Q^2). \quad (3.9)$$

Now the sum over the events has been completely absorbed into the definition of the interpolated weights. These can be calculated in a single run of the event generator and be stored efficiently. The calculation of the cross section has become a simple sum over the grid points and thus is much faster for a large number of events. The approach can easily be extended to histogrammed data like differential cross sections

by defining the observable bins and computing one weight $W_{i,j,k}^{(p),(s),(b)}$ for each bin b . However, unlike the full event record, the weight grid is restricted to the observable it was constructed for and cannot be used to calculate any other values.

While the variation of the PDF and α_s is still straightforward, scale variation is slightly more complicated because the weights themselves depend on the scale choices. Nevertheless, it is possible to vary the scales without too much effort, using DGLAP evolution. The precise procedure is explained in [4].

4 The considered process: Higgs production through gluon fusion

The Englert-Brout-Higgs-Guralnik-Hagen-Kibble mechanism (commonly Higgs mechanism) explains the non-zero masses of the gauge bosons in the standard model. It has been developed in the 1960s with important contributions coming from several people [39–44]. It invokes the process of spontaneous symmetry breaking and evades the Goldstone theorem. In the development of the standard model, the Higgs mechanism played a key role and ever since the discovery of a Higgs boson in 2012 by ATLAS [8] and CMS [9] at the LHC it has received wide approval.

In this thesis, the considered process is the production of a Higgs boson through gluon fusion. Accurate theoretical predictions of the differential observables are crucial to the analysis of the properties of the discovered particle. This chapter provides a description of the gluon fusion process and its features. Section 4.3 addresses the distribution of the transverse momentum in particular.

4.1 Gluon fusion at the LHC

Although there are other possible production mechanisms in the Standard Model, gluon fusion is the main process at the LHC, with an expected cross section of $\approx 50 \text{ pb}$ at a center of mass energy of $\sqrt{s} = 14 \text{ TeV}$ and a Higgs mass of 125 GeV [45]. It proceeds through a triangular loop of heavy quarks (mainly top quarks as the Higgs coupling scales with the quark mass) as is shown in Figure 4.1.

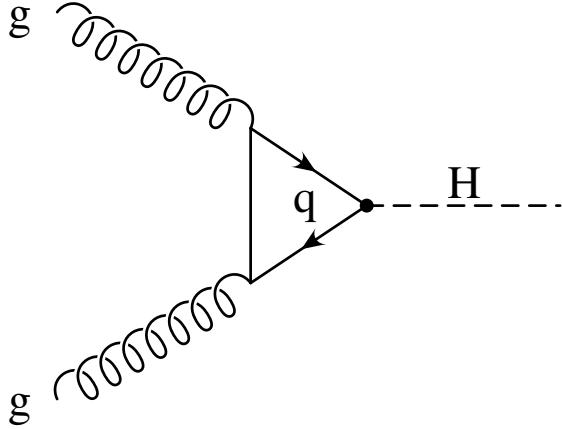


Figure 4.1: Higgs production through gluon fusion.

In the narrow-width approximation, the leading order cross section is given by [46]

$$\sigma_{\text{LO}}(pp \rightarrow H) = \sigma_0^H \tau_H \frac{d\mathcal{L}^{gg}}{d\tau_H}, \quad (4.1)$$

where $\tau_H = M_H^2/s$ is the Drell-Yan variable and $d\mathcal{L}^{gg}/d\tau_H$ is the gluon luminosity. The partonic cross section σ_0^H can be written as

$$\sigma_0^H = \frac{G_F \alpha_s^2(\mu_R^2)}{288\sqrt{2}\pi} \left| \sum_q \frac{3}{2\tau_q} \left[1 + \left(1 - \frac{1}{\tau_q} \right) f(\tau_q) \right] \right|^2, \quad (4.2)$$

with the form factor

$$f(\tau_q) = \begin{cases} \arcsin^2(\sqrt{\tau_q}), & \tau_q < 1, \\ -\frac{1}{4} \left[\ln \frac{1+\sqrt{1-\tau_q^{-1}}}{1-\sqrt{1-\tau_q^{-1}}} - i\pi \right]^2, & \tau_q > 1, \end{cases} \quad (4.3)$$

where G_F denotes the Fermi coupling constant and $\tau_q = m_H^2/4m_q^2$. The gluon

luminosity takes the form

$$\frac{d\mathcal{L}^{gg}}{d\tau_H} = \int_0^1 dx_1 dx_2 g(x_1, \mu_F^2) g(x_2, \mu_F^2) \delta(x_1 x_2 - \tau_q) \quad (4.4)$$

with $g(x, \mu_F^2)$ denoting the gluon PDF.

The QCD corrections are composed of virtual corrections to the vertices and propagators, real gluon radiation in the initial state and the contributions of the subprocesses $gq \rightarrow Hq$ and $q\bar{q} \rightarrow Hg$. Exemplary diagrams for the corrections are shown in Figure 4.2. The full NLO cross section has been calculated in [47–49]. They increase the cross section by a factor of 1.5 to 1.7.

In the limit where the top quark has infinite mass, $m_t \rightarrow \infty$, the form factor takes the value $\frac{4}{3}$. This allows for an analytical expression of the corrections [48]. This approximation can be considered as an extension of the Standard Model, where the Higgs boson couples directly to gluons, known as effective Higgs coupling (cf. fig. 4.3). The effective Lagrangian for Higgs gluon interaction can be written as [50]

$$\mathcal{L}_{\text{eff}}^{ggH} = -\frac{1}{4v} C_1 G_{\mu\nu}^a G^{a\mu\nu} H, \quad (4.5)$$

where v is the Higgs vacuum expectation value, $G_{\mu\nu}^a$ is the gluon field strength tensor and H is the Higgs field. The coefficient C_1 , in the $\overline{\text{MS}}$ scheme, is given by

$$C_1 = \frac{-1}{3\pi} \left\{ 1 + \frac{11\alpha_s}{4\pi} + \left(\frac{\alpha_s}{\pi} \right)^2 \left[\frac{2777}{288} + \frac{19}{16} \log \left(\frac{\mu^2}{m_t^2} \right) \right. \right. \\ \left. \left. + n_f \left(-\frac{67}{96} + \frac{1}{3} \log \left(\frac{\mu^2}{m_t^2} \right) \right) \right] + \mathcal{O}(\alpha_s^3) \right\}, \quad (4.6)$$

where the number of active flavors should be set to $n_f = 5$. According to [50], at LO this approximation is accurate within 5 % for $m_H \approx 150$ GeV (which is close to the measured value $m_H \approx 126$ GeV) and improves at NLO. All calculations in this thesis are based on effective Higgs coupling.

Besides the basic process, the fully differential NLO cross sections are available for $H + 1$ jet [51, 52], $H + 2$ jets [53, 54] and $H + 3$ jets [55]. A fully differential

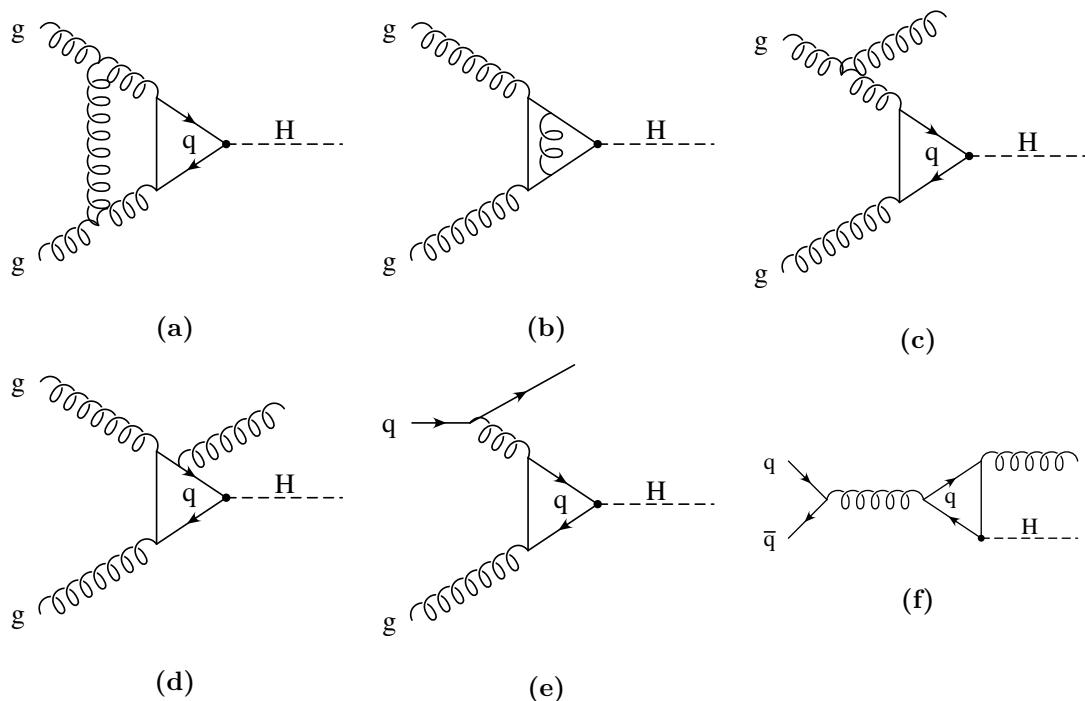


Figure 4.2: Example diagrams illustrating the QCD corrections to the process $pp \rightarrow H$: (a), (b) virtual corrections; (c), (d) real emission of a gluon; (e) $gq \rightarrow Hq$; (f) $q\bar{q} \rightarrow Hg$.

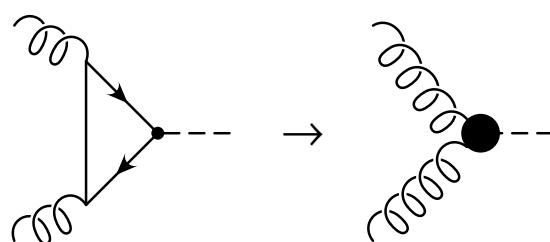


Figure 4.3: Effective Higgs coupling.

NNLO calculation exists for $H + 0$ jets production [56, 57] and substantial progress has been achieved towards an NNLO calculation of the $H + 1$ jet cross section [58].

4.2 Leptonic Higgs decay

In an experiment, one would never observe the Higgs boson directly but rather reconstruct it from the measured properties of its decay products. We want to model this situation by simulating the Higgs boson decay. There are several possible decay channels. One has to keep in mind that the Higgs coupling is proportional to the particle masses, so that it will decay into the heaviest possible particles. Assuming a Higgs mass of $m_H = 126\text{ GeV}$, the most relevant decay products are $q\bar{q}$ (where q denotes a bottom or charm quark), WW , ZZ , $Z\gamma$, $\gamma\gamma$, gg and $\tau^+\tau^-$ [59]. The decay into photons or gluons is only possible through intermediate loops. The studies leading to the discovery of the Higgs boson at the LHC relied primarily on the decay modes $H \rightarrow \gamma\gamma$, $H \rightarrow ZZ$ and $H \rightarrow WW$.

For the purpose of this thesis, the decay $H \rightarrow \tau^+\tau^-$ is considered, which has a branching ratio of approximately 6 % [60]. The Feynman diagram is shown in fig. 4.4. It would be possible to simulate the other decay channels as well, however, this would only complicate the analysis unnecessarily. The leptonic decay is the easiest one and closely resembles the Drell-Yan process. There have been searches for $H \rightarrow \tau\tau$ events in the LHC data and both ATLAS [61] and CMS [62] have published evidence for this type of decay. It also allows for the observation of additional jets that are produced in the initial state and are separated from the Higgs decay products. The further decay of the tau leptons, which would naturally occur in the experiment, will not be considered here.

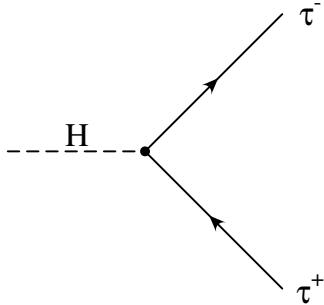


Figure 4.4: Higgs decay into two τ leptons.

4.3 The transverse momentum of the Higgs boson

The transverse momentum distribution of the Higgs boson is one of the most interesting observables in Higgs production. It provides a powerful test of the standard model once the statistics of the experimental results become suitable. In the following, we will briefly study the distribution in the gluon fusion process, where the Higgs boson is produced along with different numbers of jets. In particular, we take a look at how the quality of the prediction is influenced by parton showers. Four separate runs have been performed: One run each for zero, one and two jets at fixed order NLO and one MC@NLO run merging up to two jets in the core process. The **Rivet** analysis system has been used to extract the transverse momentum of the Higgs boson from the events. In the multijet merged run, the cases of at least zero, one or two jets have been distinguished and sorted into different histograms. Thus, we obtain inclusive observables that are comparable to the fixed order results. **SHERPA** has been used for all calculations and the **MCFM** library [63] has been interfaced for the 2-jet process. For the fixed order calculations, both the renormalization and the factorization scale have been set to the transverse mass of the Higgs boson. Final state jets have been extracted by the **FastJet** library [64] using the anti- k_t algorithm [65] with a radius parameter $R = 0.4$ and a p_\perp -cut of $p_\perp > 20 \text{ GeV}$. All the resulting histograms have been normalized to 1, so that the comparison is not affected by differences in the scale definitions between the fixed order and the merged runs. As we want to do a qualitative study rather than a quantitative one, this is no big restriction. For the same reason no uncertainties are shown in the plots. More

detailed studies can be found in the relevant literature, cf. for example [66, 67] or [45, 59, 60].

Figure 4.5 compares the fixed order NLO and the merged MC@NLO results in the case of no jets. At NLO the transverse momentum of the Higgs boson arises solely from real gluon emissions as the LO process does not have any transverse parts. The splitting leading to the real emissions is divergent in the soft and collinear limits which correspond to low transverse momenta. Therefore, in fig. 4.5, we see that the cross section diverges towards low p_{\perp} . The multijet result behaves completely different in the low p_{\perp} region and shows no divergence. In this case, the cross section is dominated by parton showers which include higher orders and are not divergent. Compared to the fixed order calculation, the cross section is much smaller in the low p_{\perp} region. As opposed to this, the cross section is amplified for $p_{\perp} \gtrsim 20$ GeV. The influence of the parton shower is negligible in this region. Instead the additional contributions come from the higher jet multiplicities that have been merged into the calculation. At high p_{\perp} , both results approach each other.

The results containing one or more jets are compared in fig. 4.6. Due to the jet cut, Higgs p_{\perp} below 20 GeV are very unlikely and present no meaningful observable, so we do not consider that case. At $p_{\perp} = 20$ GeV, when the Higgs boson recoils against the jet, the cross section diverges at NLO. Similar to the previous situation, the parton shower fixes the divergence and produces a smooth distribution. At high p_{\perp} the merged run gives a higher cross section, this time the additional contributions stem from the 2-jet process.

With two additional jets, the fixed order and the showered result become very similar, cf. fig. 4.7. The core process now is the same in both cases. Higher multiplicities in the MC@NLO result are generated only by the parton shower. The influence of the shower, though, is negligible.

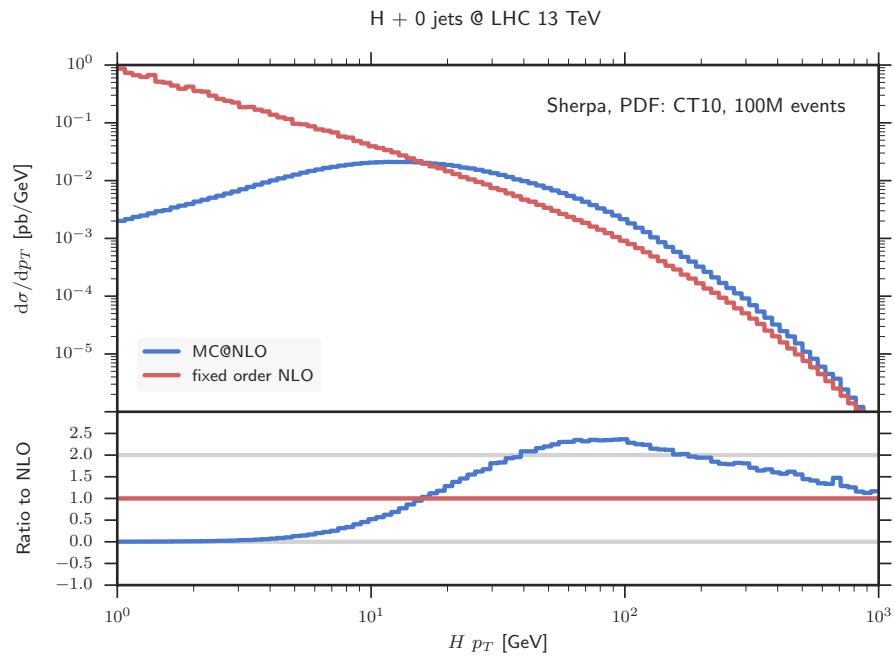


Figure 4.5: Comparison of the Higgs transverse momentum distribution between an inclusive fixed order NLO calculation and a multijet merged parton shower matched MC@NLO calculation with up to 2 jets. Note how the MC@NLO result does not diverge in the low p_{\perp} limit.

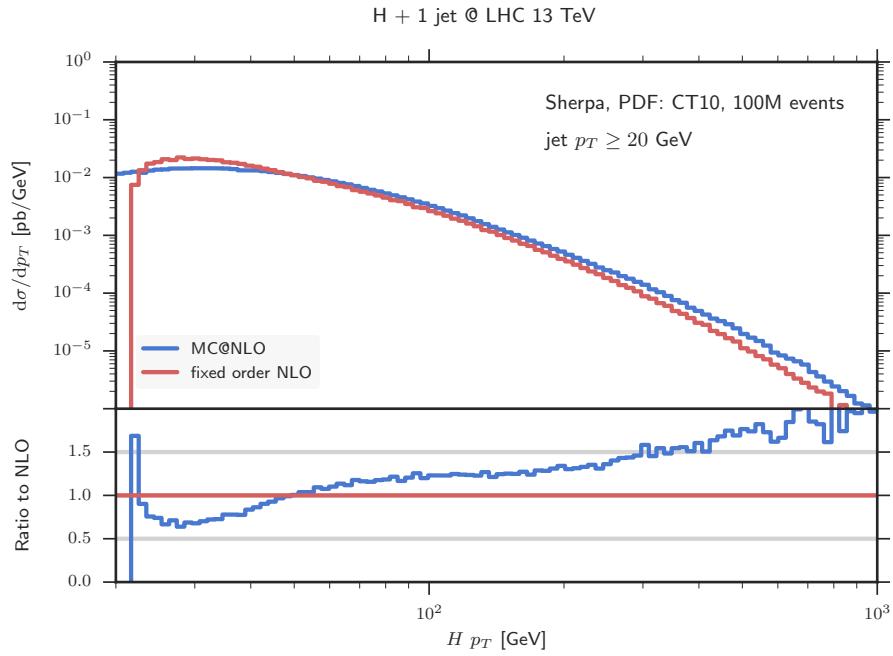


Figure 4.6: As in fig. 4.5 with at least one anti- k_t jet with $p_\perp \geq 20$ GeV.

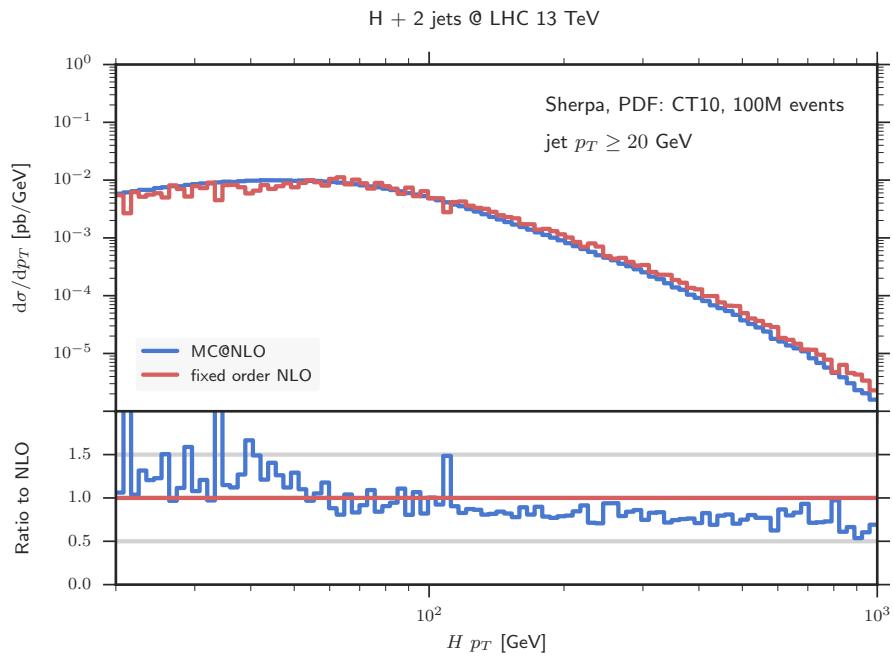


Figure 4.7: As in fig. 4.6 with at least 2 jets.

5 Validation of the interpolation method

In the following, the interpolation method used by `MCgrid` is validated for the processes $pp \rightarrow H + (0, 1, 2)$ jets at the 13 TeV LHC, computed at NLO. Thereto, reference distributions for different observables are generated using the `SHERPA` event generator and compared to the distributions obtained by convoluting a grid with the respective PDF. Additionally, the results from `APPLGRID` and `fastNLO` are compared to each other. All grids are filled using the central value of the CT10 PDF set [12]. The examined observables are the transverse momenta p_\perp of the Higgs boson and the τ leptons, respectively, the rapidity y of the Higgs boson and the pseudorapidity η of the τ leptons. The projection of the observables into histogram bins is accomplished by the `Rivet` analysis system. Final state jets are extracted by the `FastJet` library [64] using the anti- k_t algorithm [65] with a radius parameter $R = 0.4$ and a p_\perp -cut of $p_\perp > 20$ GeV.

The first validity test will check whether the grids are able to reproduce the distributions when they are filled with the same events as the reference histograms, i.e. when no parameter variation is performed. This will also determine the interpolation accuracy. Subsequently, the cases where the scale factors and/or PDFs of the grids are changed *a posteriori* will be compared to reference distributions where these parameters have been set explicitly.

5.1 The distribution of parton momenta

`APPLGRID` and `fastNLO` do not use the momentum fraction x and the factorization scale Q^2 directly in their grids. Instead, they provide transformations that are supposed to achieve better coverage of the values. In the following, we will concentrate on the x distribution, which is more crucial to the number of grid points needed. The functions provided by `APPLGRID` are:

$$f_0(x) = \log\left(\frac{1}{x} - 1\right) \quad (5.1)$$

$$f_1(x) = -\log(x) \quad (5.2)$$

$$f_2(x) = \sqrt{-\log(x)} \quad (5.3)$$

$$f_3(x) = -\log(x) + 5 \cdot (1 - x). \quad (5.4)$$

`fastNLO` only provides the functions $f_1(x)$ and $f_2(x)$. To be used in a grid, the functions are divided into equal-sized bins. In order to avoid empty bins, the limit values are determined in a separate “phase space run” before the actual fill run.

The functions (normalized to the domain $[0, 1]$ for comparability) are shown in fig. 5.1. All transformations increase the point density in the low x region, where most events should fall into. Compared against f_1 , the other functions also accomplish a higher point density in the high x region. Some observables in specific processes might benefit from this.

We can look at the actual x distribution in the process considered in this thesis. In fig. 5.2 it is plotted for one of the gluons involved in the process $gg \rightarrow H + j$ at leading order for a center-of-mass energy of $\sqrt{s} = 13$ TeV. For comparison, the respective distribution for the functions f_0 to f_3 is also shown. In the bare distribution, the number of events per bin increases rapidly towards low x . It is obvious that the reproduction of the low x region is poor for this linear binning. We expect that for some $x > 0$ the number of events approaches zero, because there has to be at least enough momentum transfer to produce the Higgs boson and the jet. To see this with linear binning, one would need a huge amount of bins. In contrast, the transformations are able to project the low x peak to a higher number of bins than the naive linear binning. Additionally, they all approach zero for a

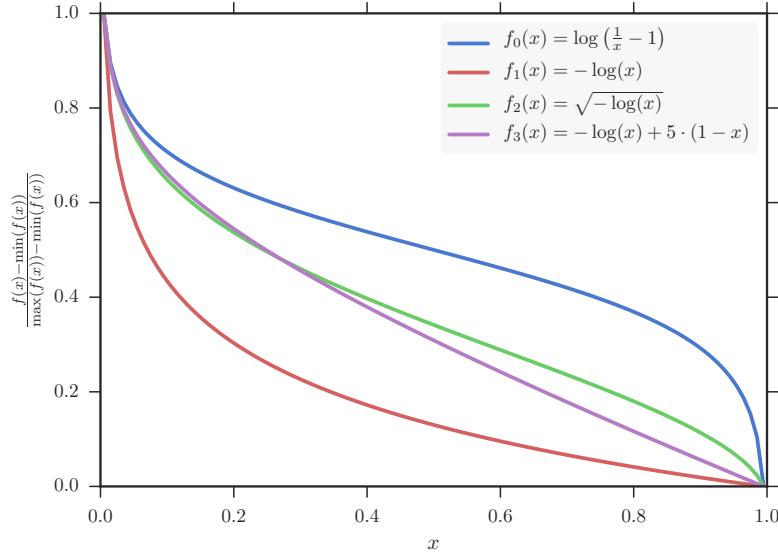


Figure 5.1: The transformations applied to the x distribution, normalized to the range $[0, 1]$.

finite value (note that high values of $f(x)$ correspond to low values of x). Due to the normalization, this happens at 1. For all transformed distributions, it should be possible to interpolate them with a reasonable number of sampling points. The function $f_1(x)$ looks most promising, as it allocates many bins for the peak region, which should be the most relevant for this process.

If we want to be more specific, we can extract the dependence of the observables on x and $f(x)$, respectively, from the generated events. This is shown in fig. 5.3 for the transverse momentum p_\perp and in fig. 5.4 for the rapidity y of the Higgs boson. We see that the rapidity heavily depends on low x values. One half of the contributions comes from values $x \leq 0.03$. Values above 0.3 are in practice negligible. The transformations reveal a substructure of the peak that is impossible to see with the linear binning. Compared to the rapidity, the transverse momentum has a higher percentage of high x values. Nevertheless, it is still dominated by the low x region.

For both observables all considered functions are a reasonable choice. Especially for the rapidity, the function $f_1(x)$ seems to be best suited. Hence, it will be the transformation used in all following grid calculations.

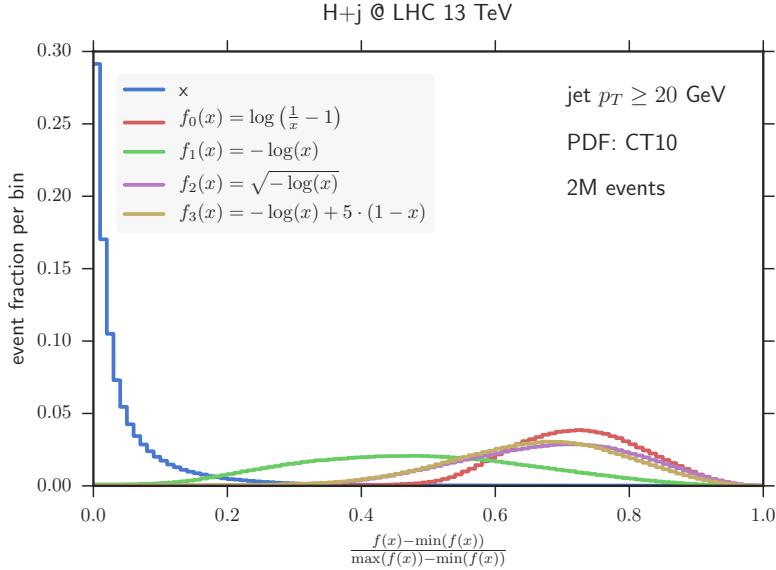


Figure 5.2: The event fraction per bin for the different transformations.

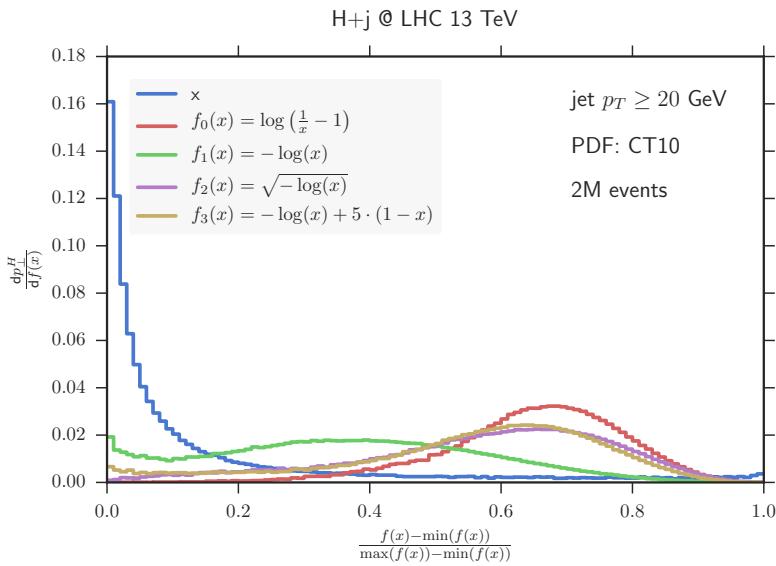


Figure 5.3: The transverse momentum p_{\perp} of the Higgs boson differential in $f(x)$. The ordinate shows the fraction per bin.

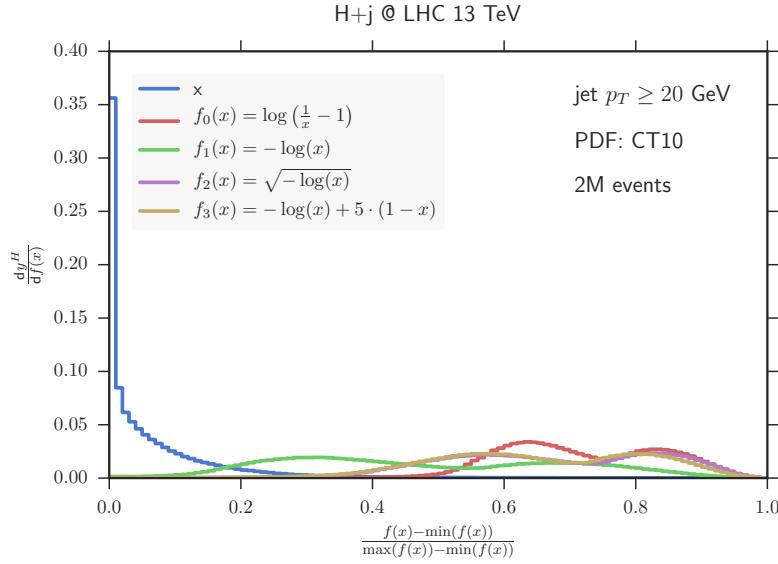


Figure 5.4: The rapidity y of the Higgs boson differential in $f(x)$. The ordinate shows the fraction per bin.

5.2 Interpolation accuracy

In this section we will prove, that the grids are able to reproduce the reference distributions up to the available interpolation accuracy. For each observable, one high precision grid and one lower precision grid is used. In the 0- and 1-jet cases, the high precision grid has 50 bins in x and the lower precision grid has 30 bins in x . In the 2-jet case, the high precision grid has 70 bins and the lower precision one has 50 bins. This is because with higher jet multiplicity, the influence of high x values increases while in all cases the same transformation is used to smooth the distribution. As we have seen in section 5.1, this transformation favors low values of x , so a higher number of grid points is needed to accurately represent the high x region. For all the following calculations, the scale parameters have been fixed to the mass of the Higgs boson. Therefore, Q^2 does not change and only one bin is used. To achieve better comparability, APPLGRID is configured to use fourth order interpolation, which is the same as is hard coded into the `fastNLO` library. Samples of 10 million events are used to fill the grids.

Figure 5.5 shows the ratio of the results obtained by convoluting the grids with

the CT10 PDF to the reference distributions for the 0-jet process. Using the high precision grid, all errors are below 0.1 %. **APPLGRID** and **fastNLO** show roughly the same accuracy. The effect of using a smaller grid is considerably bigger for the p_{\perp} distributions than for the rapidity distributions. This can be understood by looking back at figs. 5.3 and 5.4 in section 5.1. There we saw, that high values of x are completely negligible for the rapidity distribution and that it can be interpolated very well by using a logarithmic transformation. The p_{\perp} distribution is still dominated by small values of x , but compared to the rapidity large x -values have a bigger influence. Thereby, the interpolation is not as optimal. Here, the smaller grid also has a more severe impact on the **APPLGRID** result than on the **fastNLO** one.

With one jet (fig. 5.6), the errors in the reproduction of the p_{\perp} become notably larger. Even with the high precision grid, **fastNLO** produces errors for individual bins of the p_{\perp} distributions, that are large compared to the other bins. The errors of the largest outliers are about 2 %. In comparison, the errors produced by **APPLGRID** with the high precision grid are of the order of 0.01 %. The main difference between the two packages that remains in the used configuration is the interpolation function. Both use a kind of Lagrangian polynomials, but the implementations differ. It might be possible, that the function used by **APPLGRID** is more appropriate in this case. Nonetheless, the reproduction of the rapidity distributions is still very good with all grids. This is because the rapidity is not much influenced by additional jets.

The case of two jets is shown in fig. 5.7. Here the grids with 50 bins produce larger errors than in the other cases. With the high precision grid, however, **APPLGRID** still allows a very good reproduction of all observables. **fastNLO**, by contrast, features large outliers with errors of several percent. This can be attributed to the statistics. Figure 5.8 proves that the reproduction is much better with a 100 million event sample, albeit still being worse than with **APPLGRID**. The problem with the $H + 2j$ process is that the event generator produces many negative weights, so that high statistics is needed to obtain a smooth distribution. For some reason, this affects **fastNLO** more than **APPLGRID**.

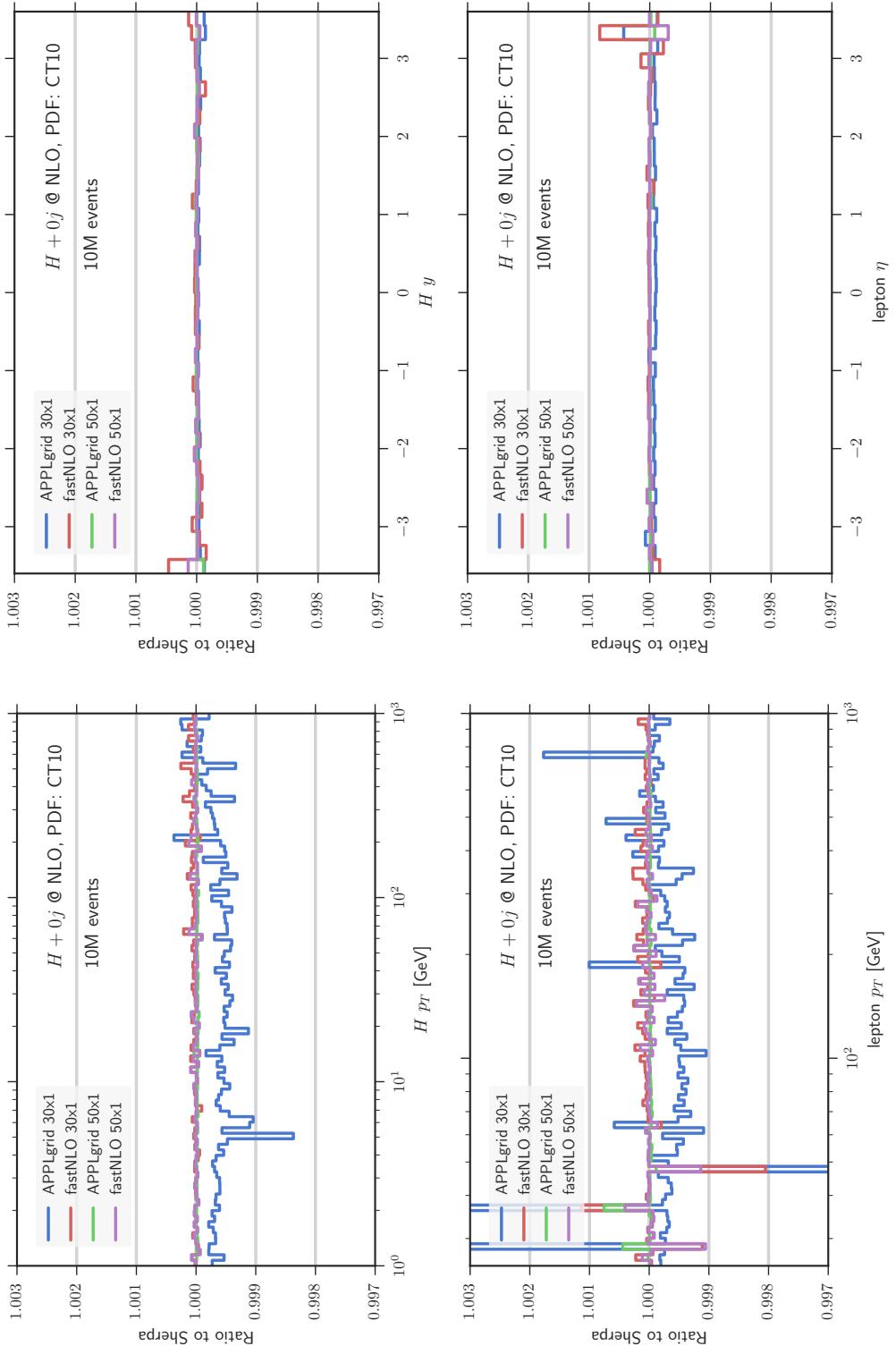


Figure 5.5: Validation of the interpolation method for the gluon fusion process. The cross section has been calculated from the interpolation grids with the same parameters as during the event generation. The results are compared to the reference distributions that have not been interpolated at all. The cross section has been evaluated differential in four different variables: The Higgs transverse momentum (upper left), the Higgs rapidity (upper right), the transverse momentum of the τ leptons (lower left) and the pseudorapidity of the leptons (lower right).

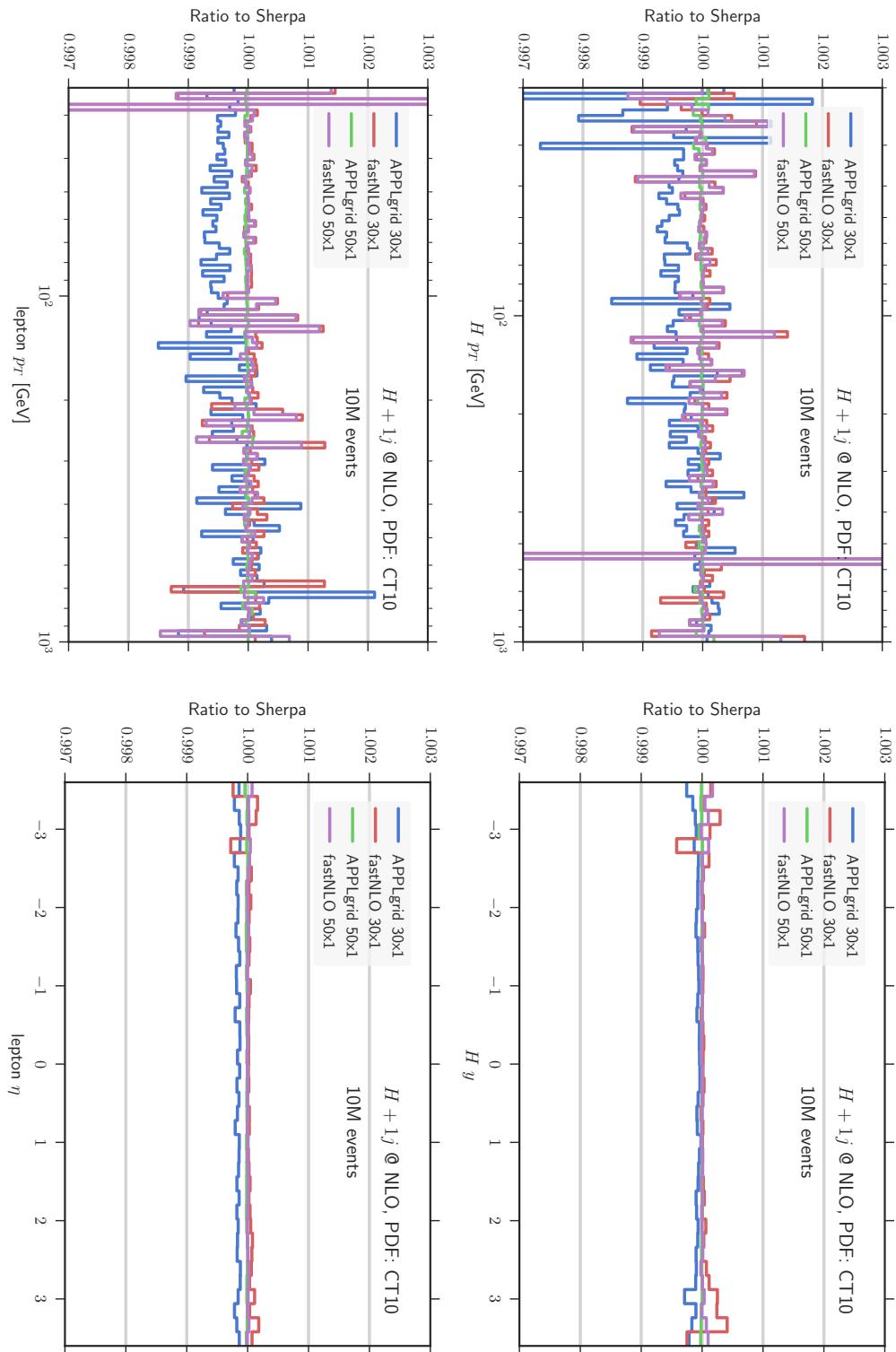


Figure 5.6: As in fig. 5.5 with one anti- k_t jet with $p_\perp \geq 20$ GeV.

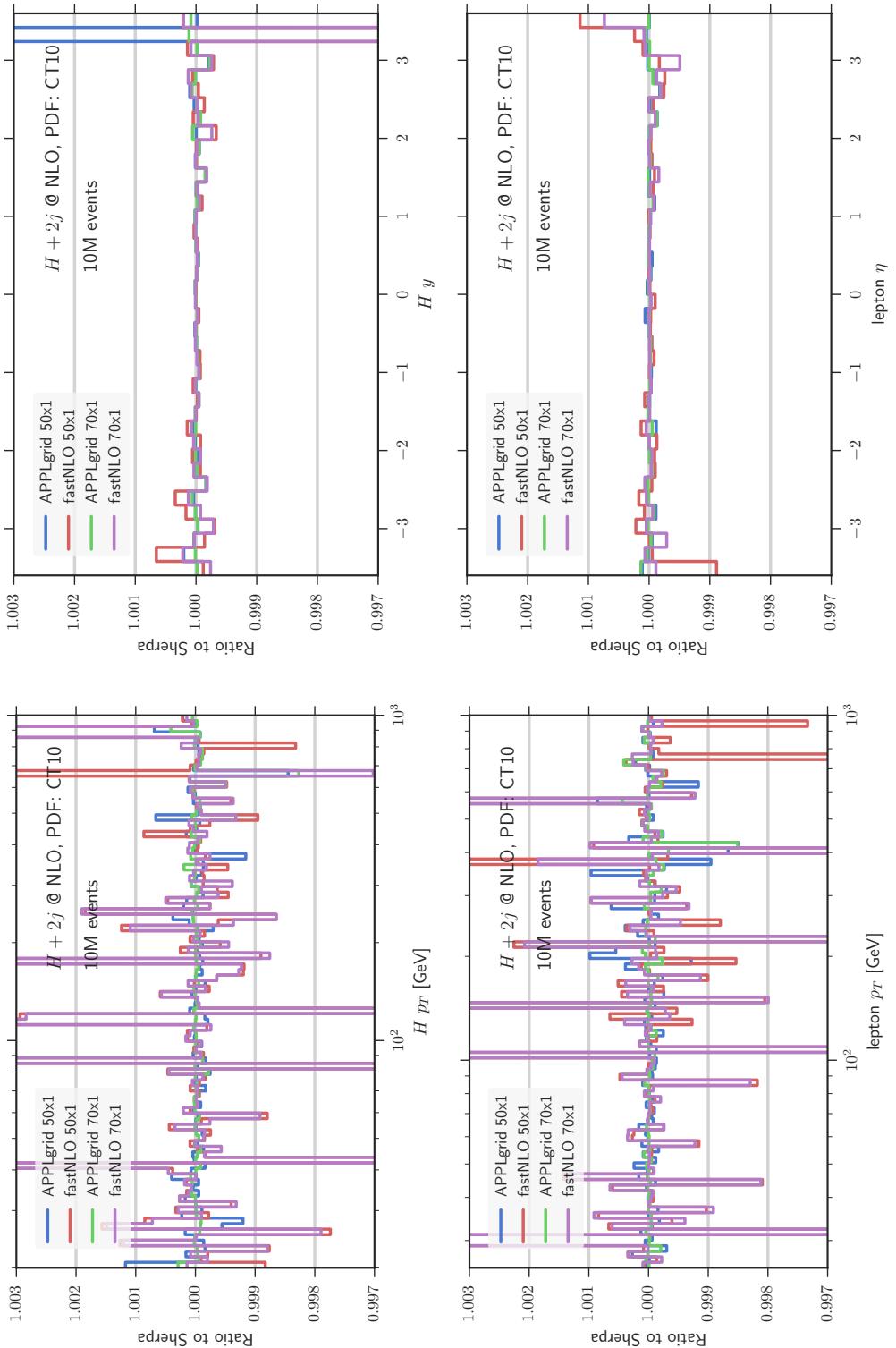


Figure 5.7: As in fig. 5.6 with 2 jets.

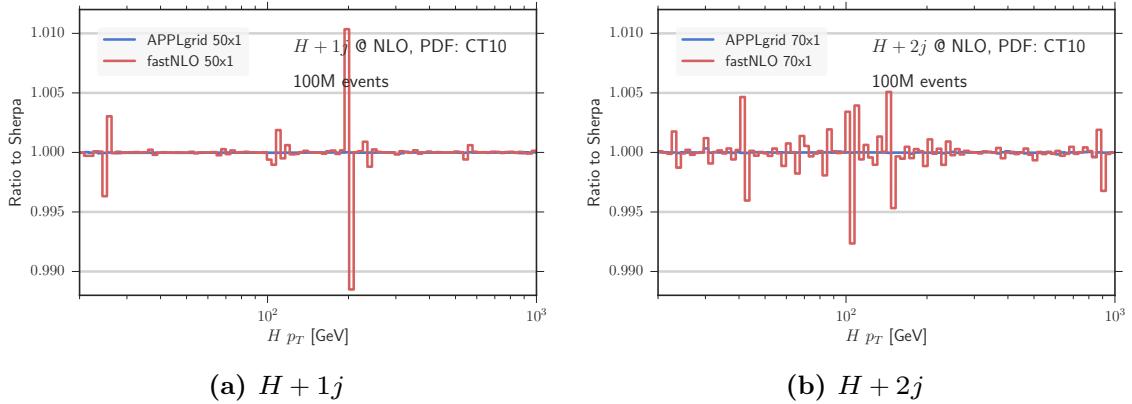


Figure 5.8: The effect of higher statistics on the interpolation. With two jets the 100 million event sample gives notably better results than the 10 million event sample in fig. 5.7. With one jet the errors are roughly the same.

5.3 Parameter variation

5.3.1 Scale factor variation

Now that we have verified that the grids produced by **APPLGRID** and **fastNLO** are able to reproduce the reference distributions up to the interpolation accuracy, we can take a look at the variation of the QCD parameters. In this section we will examine the results obtained by varying the renormalization and factorization scales. **APPLGRID** and **fastNLO** both have methods implemented that allow to change the scales when calculating NLO cross sections. There are different approaches to this. The original method used by **APPLGRID** is to apply the renormalization group equation for the renormalization scale and calculate the LO DGLAP splitting functions using **HOPPET** [68] to vary the factorization scale. **fastNLO** originally did not allow the use of **HOPPET** and instead stored individual grids for each desired factorization scale. This approach is not as flexible and leads to larger grid files but the calculation of the cross section is much faster. However, since version 2.3 **fastNLO** can also be used in combination with **HOPPET**. Another method, called “flexible-scale table”, is also implemented in **fastNLO**. It stores fully scale-independent weights and allows for arbitrary and independent variation of the scale factors without the need of splitting functions. As this feature is not yet implemented in **Mcgrid** (but will be in a future release), the first method is used in the following calculations.

The reference histograms are again generated with Sherpa using the CT10 PDF. One central scale $\mu_R = \mu_F = m_H$ and two additional scales 2μ and $\frac{1}{2}\mu$ are used. During the central scale run, grids for the transverse momentum of the Higgs boson are filled by **APPLGRID** and **fastNLO** using an MCgrid-enabled **Rivet** analysis. This is done for Higgs production with zero and one jets using an event sample of 100 million events in each case. In figs. 5.9 and 5.10 the reference distributions are compared to the results from **APPLGRID** and **fastNLO** in the 0-jet case. We observe a strong scale dependence, indicating that higher order terms entail large corrections. This turns out to be true [50, 69]. It can be seen, that the accuracy of the reproduction is very good in both cases. The discrepancies at low p_\perp in fig. 5.9 are due to an insufficient phase space run (the first ten million events have been used), meaning that during the fill run x -values emerged that were not expected by **APPLGRID**. The **fastNLO** grid was prepared with the same phase space run and obviously it responds to these events in a different way resulting in a precise reproduction throughout the range of considered values. Using a larger phase space run, the inaccuracies with **APPLGRID** would of course vanish.

In the 1-jet case, shown in figs. 5.11 and 5.12, the scale dependence is more complicated. Still, **APPLGRID** is able to reproduce all three scales at the permille level. **fastNLO**, on the contrary, shows an unexpected behavior. There are systematic deviations that increase towards high transverse momenta. As the error is definitely not caused by statistical fluctuations and because the central scale is reproduced very well, there is probably a mistake in the implementation of the evolution. A similar behavior can be observed with **APPLGRID** as well, when the 2-jet case is considered. Therefore, this does not seem to be a problem of **fastNLO** alone. This problem is object of further investigations.

5.3.2 Reweighting to a different PDF

In addition to the variation of the scale factors, it is possible to change the PDF as well. As an example, the transverse momentum of the Higgs boson is considered again. Grids that have been filled with the CT10 PDF are convoluted with the central value of the NNPDF3.0 set *a posteriori*. They are compared to the reference distribution, that has been produced by **SHERPA** using NNPDF3.0 explicitly, at three

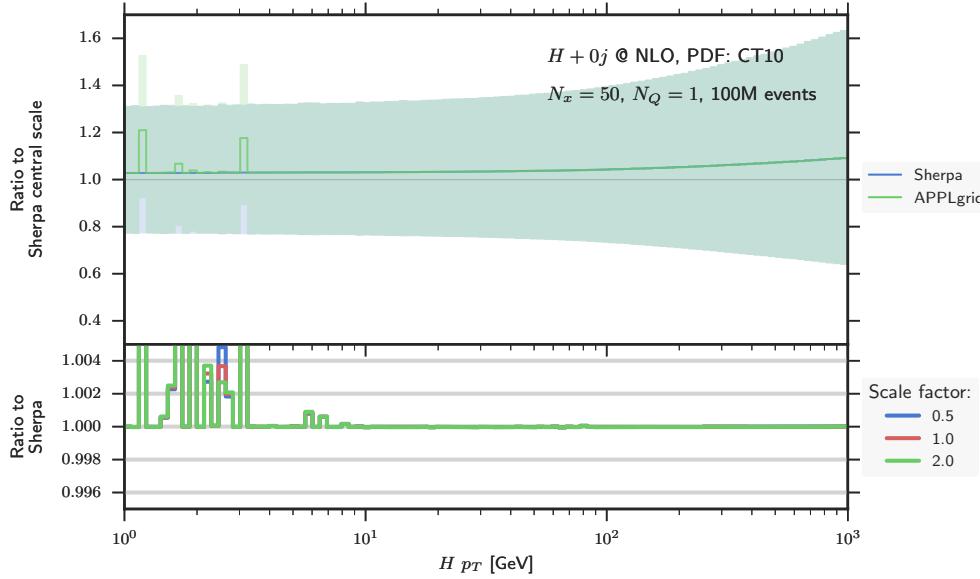


Figure 5.9: Demonstration of *a posteriori* scale factor variation with APPLGRID for $H + 0$ jets. The blue band in the upper plot shows the reference result from SHERPA and the green band shows the reproduction with an interpolation grid filled using the central scale. In both cases the central value of the variation is shown as a line. The errors at low p_\perp are not due to problems with the interpolation, more details in the text.

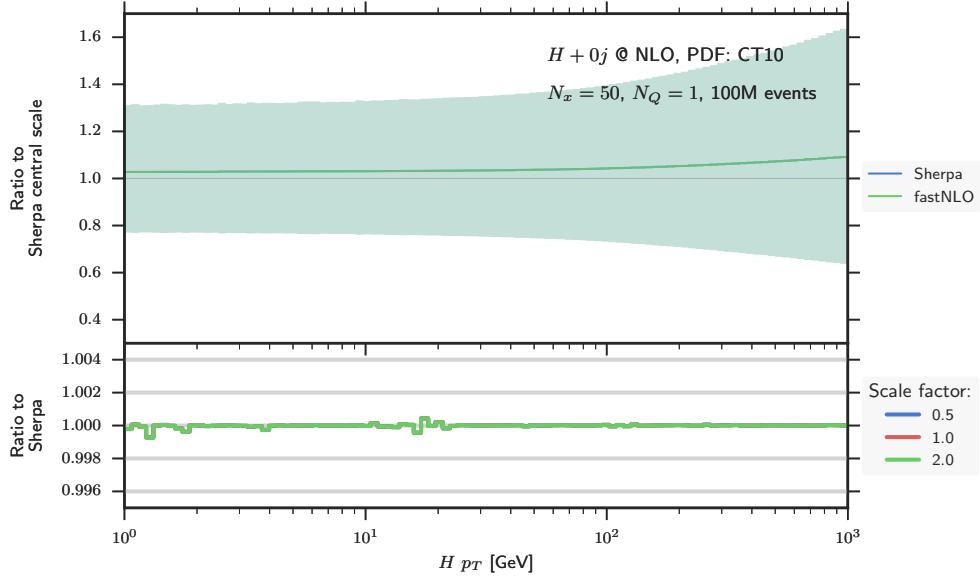


Figure 5.10: As in fig. 5.9 with fastNLO.

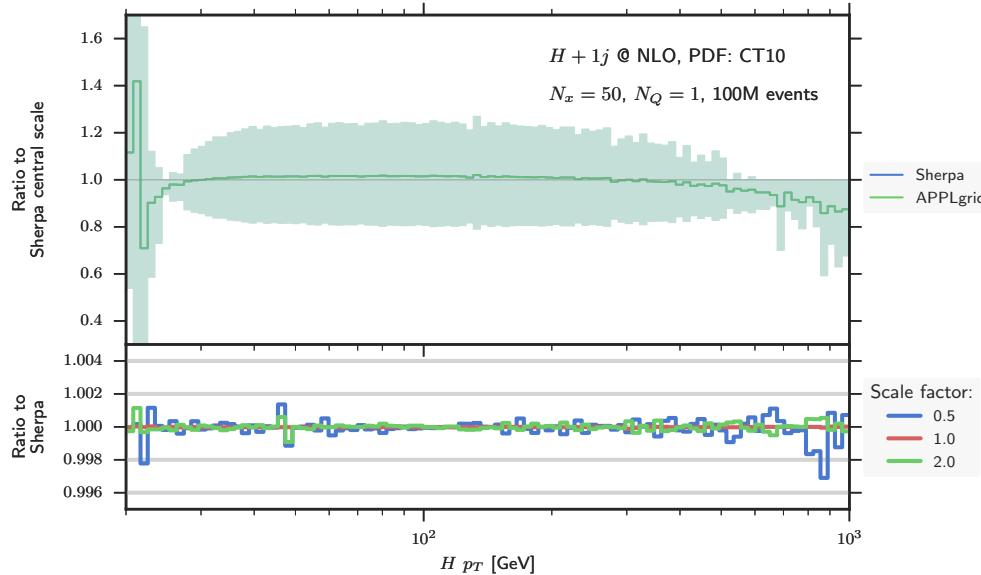


Figure 5.11: As in fig. 5.9 for $H + 1$ jet.

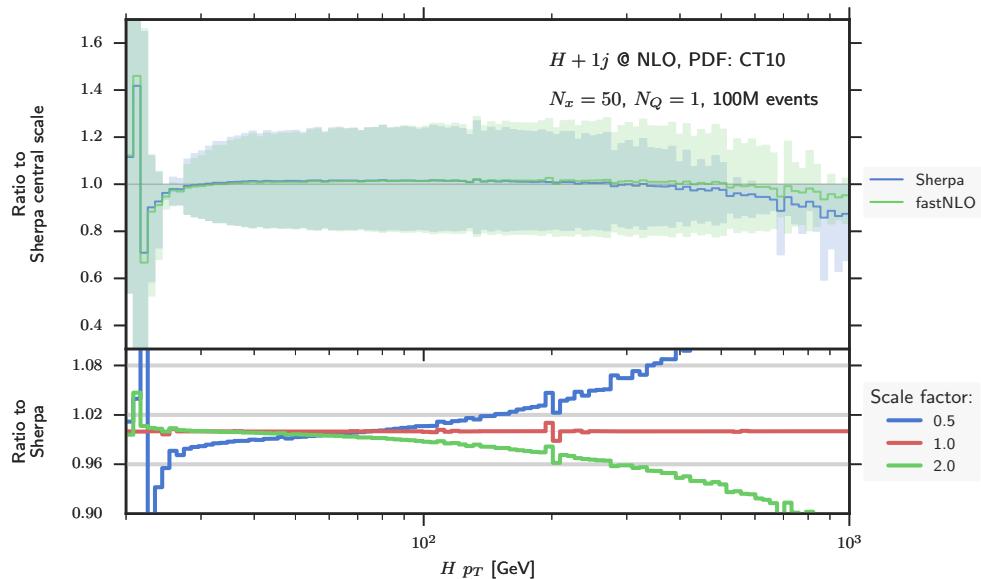


Figure 5.12: As in fig. 5.10 for $H + 1$ jet. See text for a discussion of the errors.

different scales. The results are shown in figs. 5.13 and 5.14 for APPLGRID and **fastNLO**, respectively. Again, we observe a very good reproduction. The magnitude of the errors is similar to the results of the previous section (cf. figs. 5.9 and 5.10). As has already been explained above, the discrepancies in the APPLGRID plot at low p_\perp originate from an insufficient phase space run that did not cover the whole x -range. They do not indicate any problems with the interpolation (which is proven by the **fastNLO** result in fig. 5.14) and are fixable.

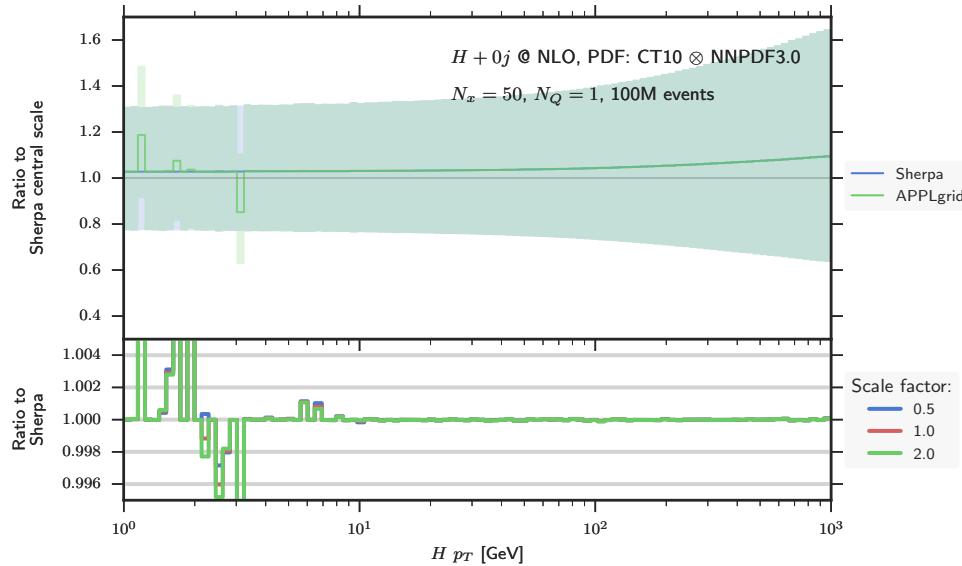


Figure 5.13: Demonstration of *a posteriori* PDF and scale factor variation with APPLGRID for $H + 0$ jets. The blue band in the upper plot shows the reference result from SHERPA and the green band shows the reproduction with an interpolation grid filled using the central scale. In both cases the central value of the variation is shown as a line. The grid has been filled with the central value of CT10 and has been convoluted with the central value of NNPDF3.0. The errors at low p_\perp are not due to problems with the interpolation, more details in the text.

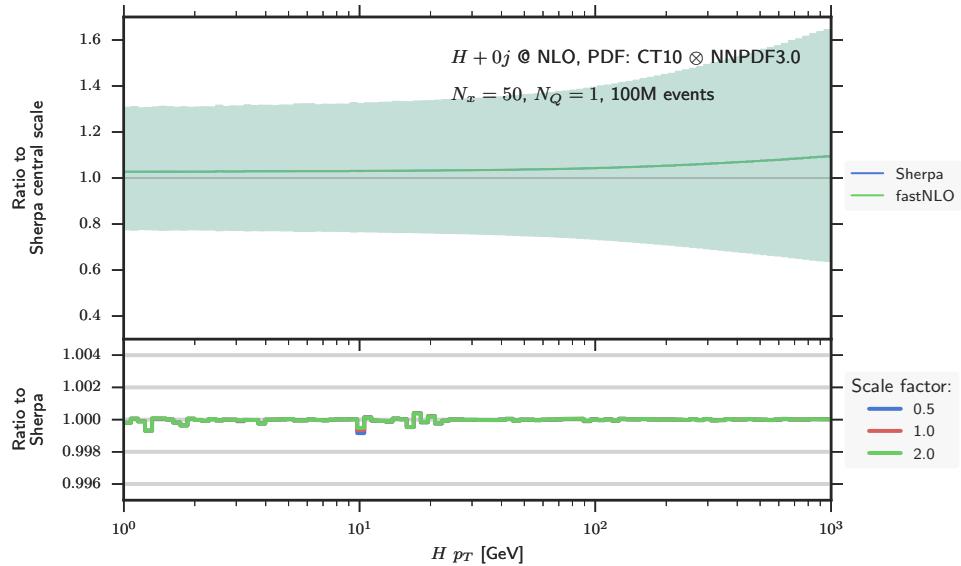


Figure 5.14: As in fig. 5.13 with fastNLO.

6 Application examples

This chapter presents two examples of application for interpolation grids. They demonstrate how they extend the number of possible calculations and allow a level of detail in the study of uncertainties that would be very expensive otherwise.

6.1 PDF uncertainty in cross section calculations

The application of the interpolation method is sensible every time a calculation has to be repeated plenty of times. This situation is given for instance, when the uncertainty from a PDF set is meant to be included in a cross section calculation. Modern PDF sets contain a large number of different samples that can be used to derive the inherent uncertainty. Having verified that the interpolation grids allow for PDF reweighting in the previous chapter, it is now justified to use them to compute the PDF uncertainty. Here we consider the NNPDF 3.0 NLO set [70], which consists of 101 samples each for 5 different values of α_s between 0.115 and 0.121. The grid that has been filled with 100 million events using the central value of the CT10 set is used to calculate a total of 505 replicas for the Higgs p_\perp in fig. 6.1. The similarity between the **APPLGRID** and **fastNLO** plots confirms the correctness of the calculation, as inaccuracies would propagate quite differently in the two implementations. Once again we see the effects of an insufficient phase space run that have already appeared in figs. 5.9 and 5.13. Another thing to observe is that the PDF uncertainty is significantly smaller than the scale uncertainty, even when combined with the error on α_s . The ratio between them is roughly $\frac{1}{6}$.

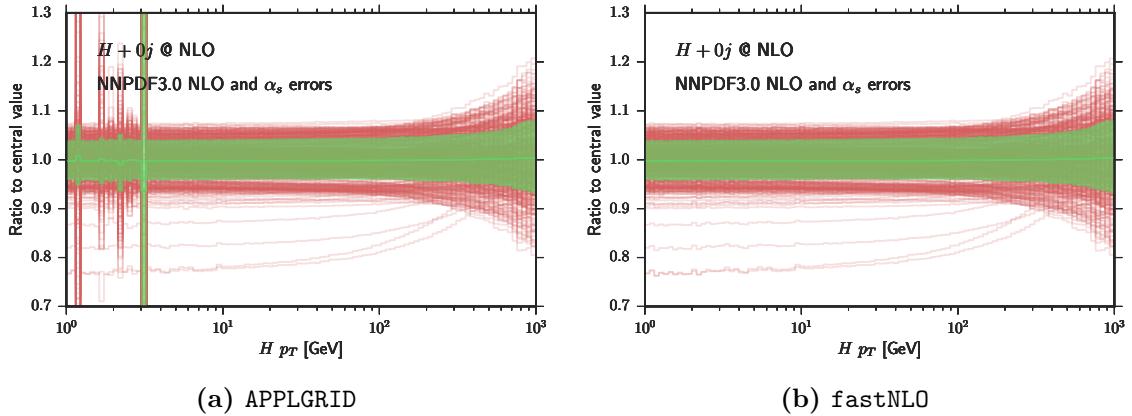


Figure 6.1: Application example of the interpolation method. The figure shows the distribution of replicas from the NNPDF3.0 NLO set including the error on α_s for the p_\perp of the Higgs boson in gluon fusion. The green area highlights the $1-\sigma$ confidence interval. The errors in the low p_\perp region of the APPLGRID plot do not indicate problems with the interpolation, this is explained in chapter 5.

6.2 Detailed scale dependence of the cross section

When one wishes to estimate the uncertainty of a fixed order calculation, a common method is to vary the renormalization and factorization scales simultaneously or independently by some factor, usually a factor of 2. This way one hopes to get a reasonable estimate of the corrections due to higher order terms. Typically, only the boundary values are calculated because of limited resources. However, using interpolation grids, any combination of scale factors can be evaluated very fast. To demonstrate this, fig. 6.2 shows the total cross section of inclusive Higgs production through gluon fusion for different combinations of scale factors, calculated using a `fastNLO` grid. Both the renormalization scale and the factorization scale are independently varied by 13 factors between $\frac{1}{4}$ and 4 resulting in a total number of 169 calculations of the cross section. We see that the dependence on the factorization scale is low whereas we observe a strong dependence on the renormalization scale.

Calculations such as this one and the example illustrated before would be extremely costly if done explicitly. If they are time-critical, explicit calculations become impossible. Interpolation tools offer much more flexibility in these cases. Especially the estimation of uncertainties can be much more differentiated.

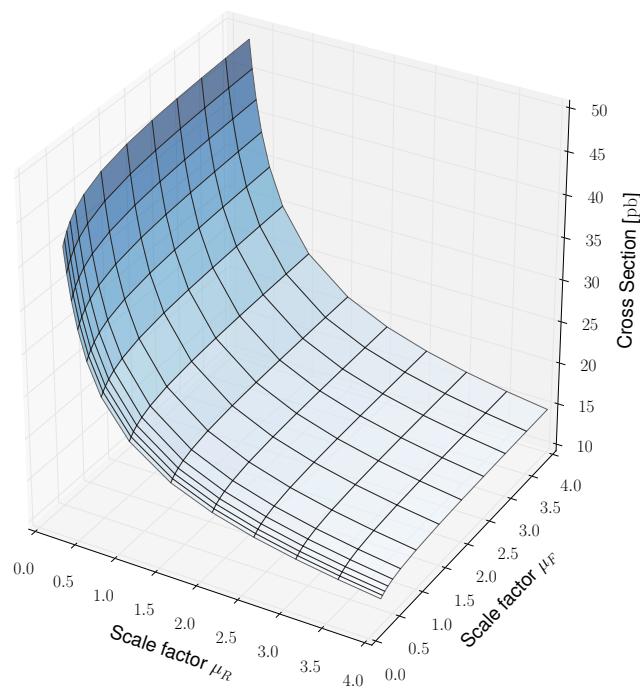


Figure 6.2: Application example of the interpolation method. The figure shows the total cross section of inclusive Higgs production at NLO as a function of the renormalization and factorization scales. The values have been generated from a `fastNLO` grid.

7 Conclusion

In this thesis, an interpolation method has been used to accelerate the variation of parameters in a fixed order NLO calculation. `MCgrid` has been used to interface two different tools, `APPLGRID` and `fastNLO`, which have been used to fill interpolation grids with the correct information. This has been performed explicitly for the example of Higgs boson production at the LHC. It could be verified that the applied method is able to achieve sub-percent accuracy in the reproduction of different observables. The possibility of *a posteriori* variation of the renormalization and factorization scales has been demonstrated. It shows no significant decrease in accuracy when no additional hard jets are considered but problems in the reproduction emerged in the cases of one and two additional jets (cf. section 5.3.1). They seem to be caused by the technique that is used to variate the scales and not by errors in the interpolation method itself. Future investigations will isolate the cause of the problem and deduce what is needed to fix it. Changing the PDF during the reevaluation of the cross section, however, has caused no further problems and has provided reproduction accuracy at permille level.

Two examples have been demonstrated that give an impression of possible applications. Global PDF fits benefit from the possibility of evaluating a large number of PDFs in cross section calculations. Without tools like `APPLGRID` and `fastNLO`, many processes could not be included in fits beyond LO. In addition to that, the interpolation tools simplify the treatment of uncertainties in theoretical predictions

based on Monte Carlo event generators.

Further studies concerning the use of **MCgrid** in the Higgs production process could include dynamically allocated scales. This case adds further complexity to the interpolation grids as the dependence on the scales has to be interpolated as well. It could not be validated yet. In a next step the support of the fixed order expansion of **MC@NLO**, which is introduced in version 2.0 of **MCgrid**, needs to be verified as well. That would pave the way for a complete inclusion of multijet merged calculations. It is a desirable goal, because merged calculations are very complex and time consuming and therefore are very well suited for a method that allows faster computation.

In section 5.1 we examined how **APPLGRID** and **fastNLO** parametrize the x -distribution to provide a better coverage of the data on a grid with equal-sized bins. Which transformation should be used depends on the considered observable. To achieve the best possible performance, one would have to check the actual x -distribution in each case. The provided transformations are obviously a compromise to cover the needs of a large number of processes. The drawback of this approach is that for some observables one needs unnecessary large grids to reliably reproduce them. There is, however, an alternative way: When performing the phasespace run prior to the fill run one could, instead of only determining the limit values of x and Q^2 , sample the whole distribution. By the use of numerical inversion, the data could then be used to provide a transformation that represents the actual distribution of x or Q^2 in the process. Thus, the bins of the grid would be filled ideally and a smaller grid would suffice to reproduce the desired observable. This would improve the overall performance of the software, as a smaller grid means less computation time and less memory consumption.

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