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Recent Developments of the fastNLO Toolkit

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The precise calculation of hadron-hadron collisions at higher orders of perturbative QCD requires a large amount of processing power. In addition, thorough analyses require that these calculations are repeated many times for different parameters. The fastNLO toolkit can be interfaced with next-to-leading order (NLO) and next-to-next-to-leading order (NNLO) Monte-Carlo programs to make these computations more efficient. Using multi-dimensional interpolation techniques, coefficient tables are produced that allow to quickly evaluate the cross section for different PDFs, values of α_s and scale choices.

These proceedings focuses on recent developments of the fastNLO framework, in particular on the increased flexibility with respect to scale variations and the new generators that are already interfaced. As an example, the flexibility of fastNLO is shown using a measurement of the strong coupling constant, where the α_s evolution is modified to refine the fitting procedure.

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1. Introduction

Very accurate theoretical predictions are crucial for modern precision measurements in high energy physics. However, such theory calculations of observables at higher orders of perturbative QCD can be very challenging and often take a very long time. In addition, it is often necessary to repeat these complex calculations for a large set of different parameters. Typical examples for such variations are:

- The comparison of precision measurements with theory are usually performed with several sets of parton distribution functions (PDFs), that are provided by different PDF fitting groups.
- The uncertainty assessment of a single PDF set can require the evaluation of the theory predictions for a number of different PDF uncertainty eigenvectors or PDF replicas. The NNPDF [1] uncertainty prescription for example requires to evaluate the sample variance on a set of 100 to 1000 different PDF replicas.
- For the estimation of the effect of missing higher orders in theory predictions, the calculations are conventionally repeated for different choices of the renormalization and/or factorization scale. For processes involving multiple scales it is often necessary to also investigate these scale variations as a function of different observables of the processes.
- The determination of theory parameters from measurements, like the value of the strong coupling constant or constraining PDFs, requires the evaluation of theory predictions for different values of these parameters. The fit procedure for PDFs involves the recalculation of theory predictions for a large number of different observables due to the parameter changes in the underlying PDFs in each step of the fitting procedure. FastNLO is used by various PDF fitting groups, like ABM [2], CTEQ-JLAB [3], CTEQ-TEA [4], HERAPDF [5], MMHT [6], or NNPDF [1].

In particular for observables like Drell-Yan and jet cross sections at hadron-hadron colliders, the evaluation of these variations using only the next-to-leading order (NLO) or next-to-next-to-leading order (NNLO) code can quickly become impractical. fastNLO [7, 8, 9] was developed to substantially reduce the amount of processing power that is needed to investigate different variations of predictions for observables in NLO or even higher-order.

1.1 fastNLO fundamentals

Perturbative QCD predictions for observables in hadron-induced processes depend on the strong coupling constant α_s and on the PDFs of the hadron(s). Any cross section in lepton-hadron or hadron-hadron collisions can expressed in terms of the strong coupling constant to the power of n, α_s^n, the perturbative coefficients $c_{i,n}$ for the partonic subprocess i, and the corresponding linear combination of PDFs from the one or two hadrons f_i, which is a function of the fractional hadron momenta x_1, x_2 carried by the respective partons. The equation describing hadron-hadron cross sections with subprocess $i = (a,b)$ for the interaction of parton a, b in particular is given by:

$$\sigma_{pp\to \mathrm{X}}(\mu_r,\mu_f) = \sum_{a,b,n} \int_0^1 dx_1 \int_0^1 dx_2 \alpha_s^n(\mu_r) c_{(a,b),n} f_{1,a}(x_1,\mu_f) f_{2,b}(x_2,\mu_f) \tag{1.1}$$

The fundamental concept behind fastNLO is to isolate the perturbative coefficients $c_{i,n}$ from the PDFs and the α_s factors and thereby convert this integration into a sum [10, 11]. This discretization introduces a set of eigenfunctions $E_k(x)$ (with $\sum_k E_k(x) \equiv 1$) around a defined number of x-values. The PDFs $f_p(x_p)$ in equation 1.1 can then be replaced by $f_p \simeq \sum_k f_p(x_k) E_k(x)$ and moved in front of the integral. The remaining integration over x to compute the cross section is turned into a sum over the n perturbative orders, i parton flavors, and all the x-nodes.

The perturbative coefficients $c_{i,n}$ can be further decomposed to describe the dependence on the renormalization and factorization scales μ_r, μ_f at NLO with $c^0_{i,n}$,$c^r_{i,n}$,$c^f_{i,n}$ and NNLO with $c^r_{i,n}r$,$c^r_{i,n}f$,$c^f_{i,n}f$:

$$\begin{aligned} c_{i,n}(\mu_r,\mu_f) \;=\; & c^0_{i,n} + \log(\mu_r) c^r_{i,n} + \log(\mu_f) c^f_{i,n} \\ & + \log(\mu_r^2) c^r_{i,n} r + \log(\mu_f^2) c^f_{i,n} f + \log(\mu_r^2)\log(\mu_f^2) c^r_{i,n} f \end{aligned} \tag{1.2}$$

For the determination of the renormalization scale variations, fastNLO allows to either use the RGE in conjunction with the leading-order matrix element, or directly store the scale-independent weights from equation 1.2. Variations of the factorization scale can be done by either storing the coefficients for a fixed set of factorization scales, by using the LO DGLAP splitting functions from HOPPET [12], or by simply storing the scale-independent weights as above.

The perturbative coefficients only need to be calculated once with very high statistical precision, with the weights describing these coefficients being stored in an interpolation table. These tables can be enriched with additional additive or multiplicative contributions to the cross sections.

It is also possible to include measurements and (un-)correlated uncertainties in a single table. When processing these tables, the summation of weights can be adapted to different PDFs, values of α_s or scale choices. This allows to quickly perform all needed variations in a fraction of the time needed to do the full calculation.

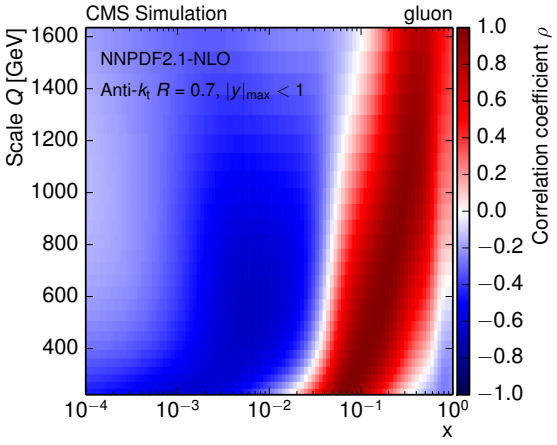

Figure 1: Correlations between the gluon PDF and the three-jet production cross section as a function of x and the scale of the process[13].

An example for an application of these techniques is shown in figure 1, which presents the correlation between the gluon PDF and the three-jet production cross section in proton-proton collision events. In order to calculate these correlations, three-jet production cross sections were evaluated for all of the 100 PDF replicas of the NNPDF 2.1 [14] PDF set within seconds. Since fastNLO provides information about the average scale that is used in each observable bin, the correlation between the cross section and the gluon PDF could be shown as a function of x and the scale of the process.

2. Recent developments

While fastNLO was already directly interfaced to some important (N)NLO generators like `NLOJet++` [15, 16, 17] or DiffTop [18], the recently developed interface to `MCgrid` [19] enables access to Monte Carlo generators like `Sherpa`[20] and the analysis code contained in `RIVET` [21].

The new fastNLO toolkit has a clean interface to implement interfaces to additional (N)NLO Monte-Carlo in order to create tables. It also provides users with simple to use interfaces in C++, Fortran and Python to read tables and calculate cross sections using existing PDFs and α_s evolution codes as provided by `LHAPDF 5/6` [22, 23] for example. For advanced users it is also possible to provide own PDFs and α_s evolution codes in C++ or Fortran that can be used in the table evaluation.

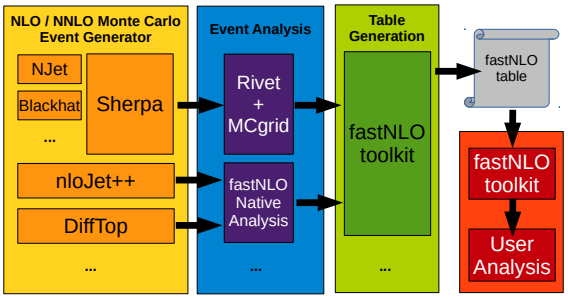

Figure 2: Overview of the fastNLO processing workflow. Several NLO and NNLO generators are directly or indirectly (via `MCgrid`+`RIVET`) interfaced to fastNLO and can be used to create interpolation tables. These tables can be used to quickly evaluate theory predictions for different PDFs, α_s or scale choices.

3. fastNLO in action

The flexibility of fastNLO with respect to the α_s evolution that is employed during the table evaluation allows to refine the fit procedure for $\alpha_s(M_Z)$ as it is used by experiments[25, 26] .

Since global PDF fits are only provided for a limited set of $\alpha_s(M_Z)$ values, the common procedure calculates the χ^2 between data and the theory predictions that are given by the α_s series. The fit result is then derived from a parametrisation (usually a simple polynomial of order 2) of the χ^2 curve.

The refined method replaces the α_s evolution code in fastNLO that is provided by `LHAPDF` with another α_s evolution code[27] that allows to freely choose the value of $\alpha_s(M_Z)$. This allows to calculate arbitrary values of $\chi^2(\alpha_s(M_Z))$ without resorting to parametrisations and enables the application of common minimization libraries to derive the central fit result and the uncertainties.

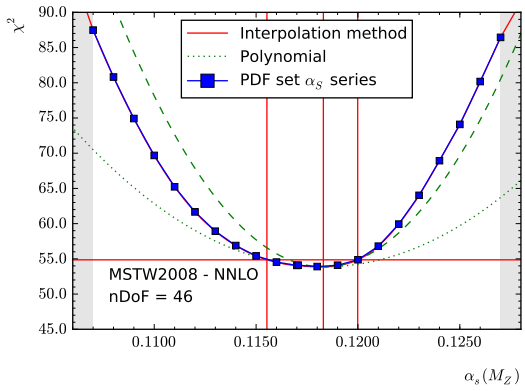

Figure 3: Comparison between the commonly used α_s fit method (green) and the refined method (red). The χ^2 is calculated from the measurement of the three-jet production cross section[13] and theory predictions (`NLOJet++` with MRST2008 PDF[24]).

As shown in figure 3, the refined method directly provides a straightforward description of the uncertainties without any ambiguities introduced by choosing some parametrisation.

3.1 Mathematical description of the refined method

Mathematically, this replacement can be described with the following set of equations. Any observable O that can be calculated by fastNLO can be expressed as:

$$O = O(\mathrm{PDF}^i(\alpha_s^{\mathrm{PDF,i}}(\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}}), M_{\mathrm{Z,i}}, Q)), \alpha_s^{\mathrm{fastNLO}}(\alpha_s^{\mathrm{fastNLO}}(M_{\mathrm{Z}}), M_{\mathrm{Z}}, Q)) \tag{3.1}$$

PDF^i is a PDF member i that is provided by a PDF fitter group together with a certain $\alpha_s^{\mathrm{PDF,i}}$ evolution for a given $\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}})$. By default, fastNLO evaluates the observable with:

$$\alpha_s^{\mathrm{fastNLO}}(\alpha_s^{\mathrm{fastNLO}}(M_{\mathrm{Z}}), M_{\mathrm{Z}}, Q) = \alpha_s^{\mathrm{PDF,i}}(\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}}), M_{\mathrm{Z,i}}, Q) \tag{3.2}$$

However for the presented method $\alpha_s^{\mathrm{fastNLO}}(\alpha_s^{\mathrm{fastNLO}}(M_{\mathrm{Z}}), M_{\mathrm{Z}}, Q)$ can be any α_s evolution code, where $\alpha_s^{\mathrm{fastNLO}}(M_{\mathrm{Z}})$ can be choosen freely. In order to guarantee perfect agreement for the observable when calculated with the exact calculation at $\alpha_s^{\mathrm{fastNLO}}(M_{\mathrm{Z}}) = \alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}})$, a correction factor k_i is defined by:

$$k_i = \frac{O(\mathrm{PDF}^i(\alpha_s^{\mathrm{PDF,i}}(\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}}), M_{\mathrm{Z,i}}, Q)), \alpha_s^{\mathrm{PDF,i}}(\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}}), M_{\mathrm{Z,i}}, Q))}{O(\mathrm{PDF}^i(\alpha_s^{\mathrm{PDF,i}}(\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}}), M_{\mathrm{Z,i}}, Q)), \alpha_s^{\mathrm{fastNLO}}(\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}}), M_{\mathrm{Z}}, Q))} \tag{3.3}$$

This correction factor is usually very small and on the permille level. The observable $\mathscr{O}_i(\alpha_s(M_{\mathrm{Z}}))$ represents an extrapolation of O calculated for a PDF member i with associated $\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}})$ to arbitary values of $\alpha_s(M_{\mathrm{Z}})$ and takes the form:

$$\mathscr{O}_i(\alpha_s(M_{\mathrm{Z}})) = k_i \cdot O(\mathrm{PDF}^a(\alpha_s^{\mathrm{PDF,i}}(\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}}), M_{\mathrm{Z,i}}, Q)), \alpha_s^{\mathrm{fastNLO}}(\alpha_s(M_{\mathrm{Z}}), M_{\mathrm{Z}}, Q)) \tag{3.4}$$

The refined method presented above calculates $\chi^2(\alpha_s(M_{\mathrm{Z}}))$ values outside the $\alpha_s(M_{\mathrm{Z}})$ range provided by the PDF fitter groups from $\mathscr{O}_i(\alpha_s(M_{\mathrm{Z}}))$, where i is the PDF member with the smallest or largest value of $\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}})$.

In order to calculate $\mathscr{O}(\alpha_s(M_{\mathrm{Z}}))$ for some arbitary $\alpha_s(M_{\mathrm{Z}})$ within the range provided by the PDF fitter groups, the PDF members a and b are used whose $\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}})$ values are closest to $\alpha_s(M_{\mathrm{Z}})$ with:

$$\alpha_s^{\mathrm{PDF,a}}(M_{\mathrm{Z,a}}) \leq \alpha_s(M_{\mathrm{Z}}) \leq \alpha_s^{\mathrm{PDF,b}}(M_{\mathrm{Z,b}}) \tag{3.5}$$

The value for $\mathscr{O}(\alpha_s(M_{\mathrm{Z}}))$ is based on a simple linear interpolation between $\mathscr{O}_a$ and $\mathscr{O}_b$:

$$\mathscr{O}(\alpha_s(M_{\mathrm{Z}})) = \mathscr{O}_a(\alpha_s(M_{\mathrm{Z}})) + (\mathscr{O}_b(\alpha_s(M_{\mathrm{Z}})) - \mathscr{O}_a(\alpha_s(M_{\mathrm{Z}}))) \cdot \frac{\alpha_s(M_{\mathrm{Z}}) - \alpha_s^{\mathrm{PDF,a}}(M_{\mathrm{Z,a}})}{\alpha_s^{\mathrm{PDF,b}}(M_{\mathrm{Z,b}}) - \alpha_s^{\mathrm{PDF,a}}(M_{\mathrm{Z,a}})} \tag{3.6}$$

The linear interpolation and the correction factors ensure a continous behaviour of $\mathscr{O}(\alpha_s(M_{\mathrm{Z}}))$ for all $\alpha_s(M_{\mathrm{Z}})$ and perfect agreement with the calculations from the α_s series provided by the PDF:

$$\mathscr{O}(\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}})) = O(\mathrm{PDF}^i(\alpha_s^{\mathrm{PDF,i}}(\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}}), M_{\mathrm{Z,i}}, Q)), \alpha_s^{\mathrm{PDF,i}}(\alpha_s^{\mathrm{PDF,i}}(M_{\mathrm{Z,i}}), M_{\mathrm{Z,i}}, Q)) \tag{3.7}$$

for $i = a, b$.

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