New features in version 2 of the fastNLO project

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Standard methods for higher-order calculations of QCD cross sections in hadron-induced collisions are time-consuming. The fastNLO project uses multi-dimensional interpolation techniques to convert the convolutions of perturbative coefficients with parton distribution functions and the strong coupling into simple products. By integrating the perturbative coefficients for a given observable with interpolation kernels, fastNLO can store the results of the time-consuming folding integrals in tables, which subsequently are used for very fast rederivations of the same observable for arbitrary parton distribution functions, different scale choices, or $\alpha_s(M_Z)$. Various tables with code for their evaluation are available for numerous jet measurements at the LHC, the TeVatron, and HERA. FastNLO is used in publications of experimental results by the ATLAS, CMS, CDF, D0, and H1 collaborations, and in all recent global PDF analyses by MSTW, CTEQ, and NNPDF. This article focuses on developments implemented in the new version 2 of fastNLO, enhancing and broadening its functionality.

1 Introduction and the fastNLO concept

Precision measurements in high energy physics reveal their full power only if they are compared to accurate theoretical predictions. For the interpretation of experimental data or the extraction or tuning of model parameters reasonably fast theory calculations are needed. For measurements defined in published cross sections, repeated computations of (almost) the same cross sections have to be performed. Typical examples where calculations have to be repeated more often for the same observable are:

- Comparisons of data vs. theory, where e.g. different sets of parton distribution functions (PDFs) are used, like those provided by the global fitting collaborations.
- Determination of the PDF uncertainty on theory predictions. As an example, the uncertainty on the cross sections arising from the NNPDF [1] PDF set require 100 to 1000 rederivations of the same cross sections where only the PDFs differ.
- Fitting of PDFs where for each step in the iterative procedure the cross sections have to be recalculated for the corresponding temporary PDF. FastNLO is used by various global PDF fitting groups, like MSTW [2], CTEQ [3], NNPDF [1], ABM [4], or HERAPDF [5].

- Determination of model parameters, or the determination of the strong coupling constant in iterative fits.
- Determination of the theory uncertainty of cross sections from missing higher orders, where conventionally the calculations are repeated for different choices of the renormalization and/or factorization scale.
- Studies of the scale dependence of the theory cross sections. For processes involving multiple scales it is not clear, which scale setting to choose.

Some observables in next-to-leading order (NLO) or even higher-order calculations can be computed rather fast like e.g. DIS structure functions. Other observables like Drell-Yan and jet cross sections, however, are very slow to compute. Especially the latter ones are the current focus of fastNLO. FastNLO provides computer code and precalculated tables of perturbative coefficients for various observables in hadron-induced processes. The calculation of the fundamental cross sections or matrix elements is performed by flexible computer code like `NLOJet++` [6, 7, 8, 9], which has been used here.

For illustrating the ideas in this document, all formulae are shown for jet production cross sections in deep-inelastic scattering. All concepts and formulae can be generalized to hadron-hadron collisions like at the LHC or the TeVatron [10].

1.1 The fastNLO concept

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 be written as the multiplication 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_a, x_b carried by the respective partons, as:

$$\sigma_{ep\to\mathrm{jets}}(\mu_r,\mu_f) = \sum_{i,n} \int_0^1 dx \alpha_s^n(\mu_r) c_{i,n}(\frac{x_{Bj}}{x},\mu_r,\mu_f) f_i(x,\mu_f) \tag{1}$$

The calculation of this cross section with reasonable statistical precision is very slow due to the necessary Monte Carlo integration of the accessible phase space. The idea of fastNLO is to separate the PDFs and the α_s factors from the perturbative coefficients $c_{i,n}$ and to convert this integration into a sum [11, 12]. This discretization introduces a set of eigenfunctions $E_i(x)$ (with $\sum_i E_i(x) \equiv 1$) around a defined number of x-values. The PDF in eq. 1 can then be replaced by $f_i \simeq \sum_i f_a(x_i)E_i(x)$ and is removed from the integral. When calculating the perturbative coefficients the nodes receive fractional contributions of each event within the x-range of each eigenfunction. The perturbative coefficients are calculated once with very high statistical precision and are stored in a *table*. 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. To respect the scale dependence, a similar procedure is employed. The multiplication of the PDF, α_s, and the perturbative factors are performed when reading the table of all $c_{i,n}$ values, which is very fast and gives the opportunity to change the PDFs and α_s as required. When calculating hadron-hadron cross sections, the two x integrations are replaced by two sums instead of only one like in the depicted DIS case.

2 New features in fastNLO version 2

Here, new features of the fastNLO version 2 are presented in comparison to the previous version 1.4 [10]. The fastNLO project comprises three main elements, the *table* format, *creator* code to create and *reader* code to read and evaluate the tables with an interface to PDFs.
A new *table* format features more flexibility and foresees to incorporate multiple additive or multiplicative contributions to the cross sections. Threshold corrections, which were already available previously for hadron-hadron induced inclusive jet production [13], higher-order calculations, electroweak corrections, or new physics contributions can be implemented in a similar way as soon as they are available. Further multiplicative correction factors like non-perturbative corrections can be stored together with their uncertainties. Also data can be included within the new table format together with their correlated and uncorrelated uncertainties.
The computation of the tables has been optimized. An automated scan to determine the covered x-range is performed first. The now flexible number of x-nodes for each analysis bin respects their different x-coverage. The scale dependence is stored as a separate array and also the interpolation of the scale nodes is optimized.
The fastNLO *reader* code for evaluating the fastNLO tables is now available in Fortran as well as in independently developed `C++` classes with an agreement of $\mathcal{O}(10^{-10})$ between the two. It is distributed in one package [14] as open source code, which is installable following the GNU autotools procedure with the only dependence on some external functionality to access PDFs like in LHAPDF [15]. Previously released tables keep their validity and can be converted into the new format.

3 The generalized concept of flexible-scale tables

A generalized concept for even more flexible tables was also released in fastNLO version 2. These are called *flexible-scale* tables and are based on two principles.
The dependence on the renormalization and factorization scales $\mu_{r/f}$ can be factorized when calculating the perturbative coefficients $c_{i,n}$, like

$$c_{i,n}(\mu_r, \mu_f) = c^0_{i,n} + \log(\mu_r)c^r_{i,n} + \log(\mu_f)c^f_{i,n}. \qquad (2)$$

This way, only scale independent weights c^0, c^r, and c^f are stored in three scale independent fastNLO tables. The multiplication of the scale dependent log terms are performed only when evaluating the table. Similarly to the α_s term in eq. 1, where $a_s(\mu_r)$ can be regarded as an arbitrary function of the scale μ_r, also the scales μ_r and μ_f can be regarded as functions of any relevant k observables s_k, like $\mu_{r/f} = \mu_{r/f}(s_1, s_2)$. FastNLO examples employ $k = 2$ since each observable needs a separate interpolation array and increases the required evaluation time.
This method gives the opportunity to store multiple possible scale definitions, like e.g. the jet momentum p_{T} and the event virtuality Q^2. When evaluating the fastNLO table it is now possible to choose any function of these two scale settings for the definition of the renormalization and factorization scale. Typical examples are e.g. $\mu_r^2 = (Q^2 + p_{\mathrm{T}}^2)/2$ and $\mu_f^2 = Q^2$, but also definitions like $\mu = s_1 \cdot \exp(0.3 \cdot s_2)$ are possible. Further, the scales can be varied independently and by arbitrary scale factors. This gives new opportunities to study the scale dependence of cross sections. The concept is also available for pp and $p\bar{p}$ calculations. For future applications, the *flexible-scale* concept is valid also for higher-order calculations like NNLO without any significant loss in speed.

4 Showcase application

Numerous fastNLO tables are available on the fastNLO website [14] for various measurements by ATLAS, CDF, CMS, D∅, H1, STAR, and ZEUS. All calculations were performed using the `NLOJet++` program [7, 8, 9], for calculating the matrix elements. A data/theory comparison of global inclusive jet data in hadron induced processes as a function of the transverse jet momentum for various center-of-mass energies is shown in fig. 1 employing the MSTW2008 PDF sets. Hadron-hadron induced processes further include 2-loop threshold corrections, which represent a part of NNLO. An updated version of this plot is available through the arXiv article [16].

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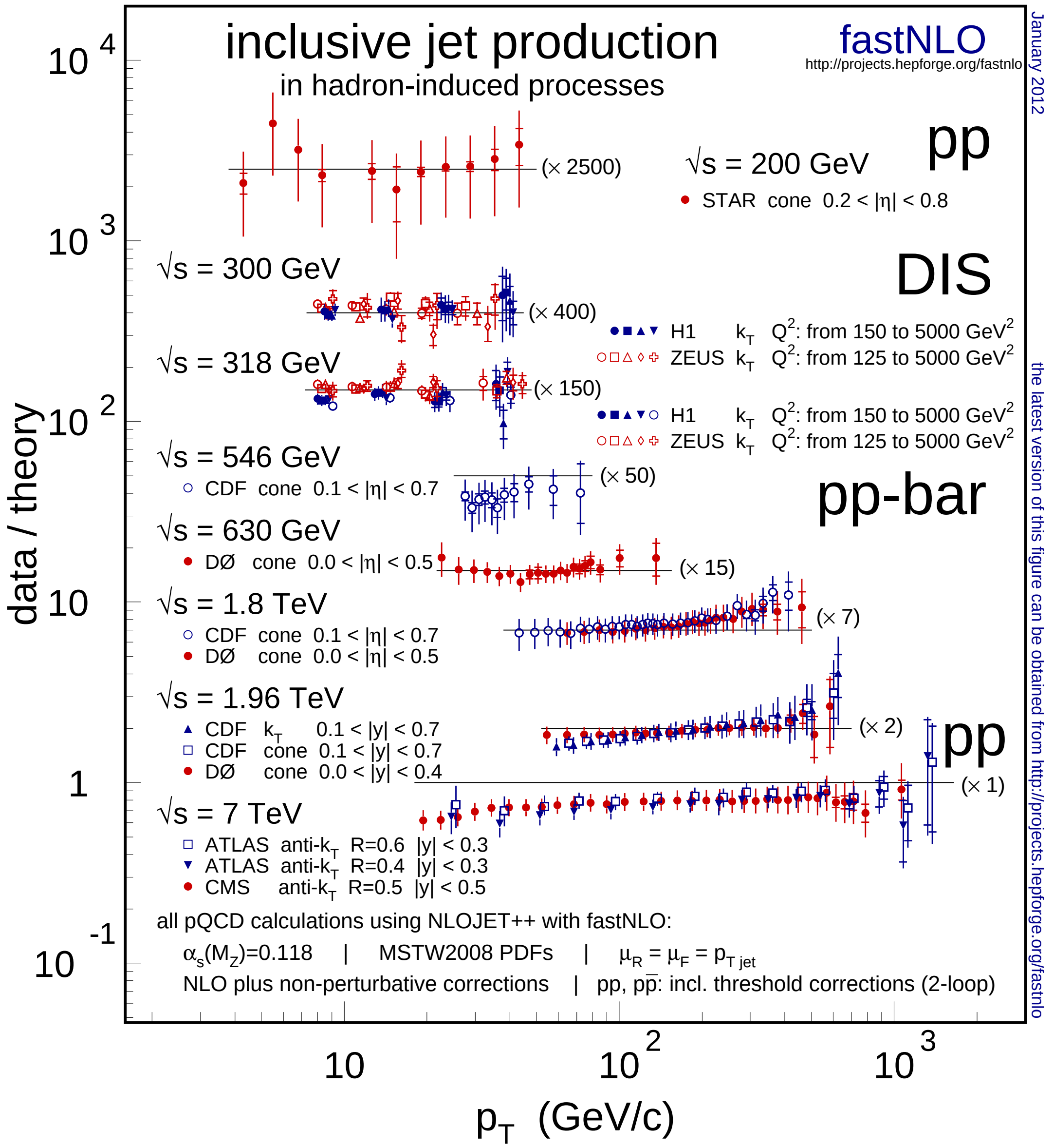

Figure 1: Ratios of data and theory for inclusive jet cross section measured in hadron-hadron collisions and in deeply inelastic scattering at different center-of-mass energies. The ratios are shown as a function of jet transverse momentum $p_{\rm T}$. The theory results are computed for MSTW2008 PDFs.