A posteriori inclusion of parton density functions in NLO QCD final state calculations

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DESY

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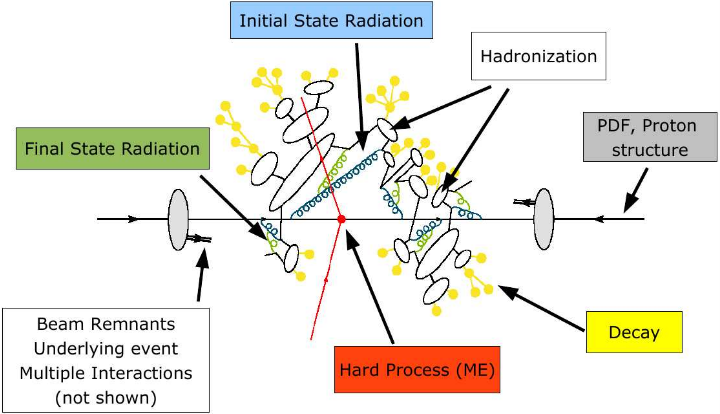
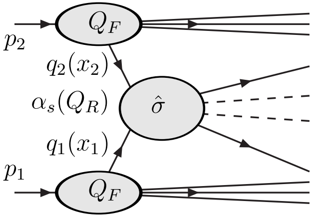
Outline

Proton-proton collision



- hard scattering can be calculated to NLO(NNLO) precision
- description of showers and non-perturbative effects comes from MC
- PDFs and strong coupling are determined from precision data (LEP, HERA, TEVATRON, . . .).

NLO QCD cross section



$$\frac{d\sigma}{dX} \sim \sum_{(i,j,p)} \int d\Gamma \alpha_s^p(Q_R^2)\, q_i(x_1, Q_F^2) q_j(x_2, Q_F^2)\, \frac{d\hat{\sigma}^{ij}_{(p)}}{dX}(x_1, x_2, Q_F^2, Q_R^2;\ S)$$

- Coupling and parton density functions are non-perturbative inputs to calculation (extracted from data)
- Perturbative coefficients are essentially independent from PDF functions due to factorization theorem

Calculating NLO cross-sections
takes a long time ($\sim$ *days*)

$\Longrightarrow$ we can split calculation into two parts

APPLGRID method

Eur.Phys.J.C66:503-524,2010.

- Step 1 (long run): Collect perturbative weights to grids .
  - binning (+ interpolation)
  - partonic sub-processes : $13 \times 13 \to \mathcal{L}$

$$d\hat{\sigma}^{ij}_{(p)}/dX \quad \to w^{(p)(l)}(x_1^m, x_2^n, Q^{2^k}) \text{ (3D-grid) } (Q_R^2 \equiv Q_F^2)$$

- Step 2 ($\sim$ 10–100 ms): Convolute grid with PDF's .
  - integral $\to$ sum
  - any coupling, pdf

$$\sum_p \sum_{l=0}^{L} \sum_{m,n,k} w^{(p)(l)}{}_{m,n,k} \left(\frac{\alpha_s(Q_k^2)}{2\pi}\right)^{p_l} F^{(l)}\left(x_{1\,m}, x_{2\,n}, Q_k^2\right) \to \frac{d\sigma}{dX}$$

Details of the method (I)

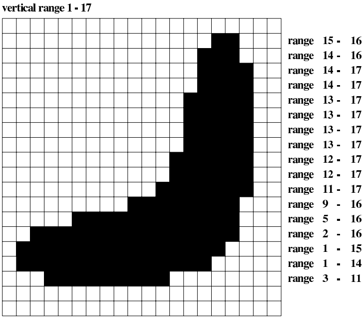
Binning

- user defined number of bins N_x and N_{Q^2} in x and Q^2
- variable transformation $(x, Q^2) \rightarrow (y, \tau)$ facilitates fine binning in regions of the phase-space where PDFs are quickly changing

$$y(x) = \ln\frac{1}{x} + a(1-x); \quad \tau(Q^2) = \ln\left(\ln\frac{Q^2}{\Lambda^2}\right)$$

  and provides the good coverage of the full x and Q^2 range
  - the parameter a allows user to control the density of points in the large x region.
  - $\Lambda \sim \Lambda_{\rm QCD}$, is user defined.

Details of the method : $x_1 x_2$ phasespace



User just defines max/min possible values of x, Q^2. The optimisation procedure finds appropriate limits for each subprocess/order/observable bin.

Details of the method (II)

Interpolation :

- user defined interpolation orders $n_y, \quad n_\tau$

$$f(x, Q^2) = \sum_{i=0}^{n_y} \sum_{\iota=0}^{n_\tau} f_{k+i,\kappa+\iota} \; I_i^{(n)}\left(\frac{y(x)}{\delta y} - k\right) \; I_\iota^{(n')}\left(\frac{\tau(Q^2)}{\delta\tau} - \kappa\right)$$

Subprocess PDFs :

$13 \times 13 \to L$ due to the symmetries of the ME weights

$$\sum_{m,n} \nu_{mn}^{(l)} \, f_{m/H_1}\left(x_1, Q^2\right) f_{n/H_2}\left(x_2, Q^2\right) \equiv F^{(l)}\left(x_1, x_2, Q^2\right),$$

“generalised“ PDFs depend on the process and the perturbative order

Final result :

$$\frac{d\sigma}{dX} = \sum_p \sum_{l=0}^{L} \sum_{m,n,k} w_{m,n,k}^{(p)(l)} \left(\frac{\alpha_s(Q_k^2)}{2\pi}\right)^{p_l} F^{(l)}\left(x_{1\,m}, x_{2\,n}, Q_k^2\right)$$

Scale dependence I

Having the weights $w_{m,n,k}^{(p)(l)}$ determined separately order by order in α_s, it is straightforward to vary the renormalisation μ_R and factorisation μ_F scales a posteriori.
We assume scales to be equal

$$\mu_R = \mu_F = Q$$

in the original calculation.
Let we introduce ξ_R and ξ_F corresponding to the factors by which one varies μ_R and μ_F respectively,

$$\mu_R = \xi_R \times Q$$
$$\mu_F = \xi_F \times Q$$

Scale dependence II

Then for arbitrary ξ_R and ξ_F we may write:

$$\frac{d\sigma}{dX}(\xi_R,\xi_F) = \sum_{l=0}^{L}\sum_m\sum_n\sum_k \Bigg\{ \left(\frac{\alpha_s\left(\xi_R^2 Q^2{}_k\right)}{2\pi}\right)^{p_{\rm LO}} \times W_{m,n,k}^{(p_{\rm LO})(l)} F^{(l)}\left(x_{1\,m}, x_{1\,n}, \xi_F^2 Q^2{}_k\right) + \left(\frac{\alpha_s\left(\xi_R^2 Q^2{}_k\right)}{2\pi}\right)^{p_{\rm NLO}}$$

$$\times\Bigg[\left(W_{m,n,k}^{(p_{\rm NLO})(l)} + 2\pi\beta_0 p_{\rm LO}\ln\xi_R^2\, W_{m,n,k}^{(p_{\rm LO})(l)}\right) F^{(l)}\left(x_{1\,m}, x_{2\,n}, \xi_F^2 Q^2{}_k\right)$$

$$-\ln\xi_F^2\, W_{m,n,k}^{(p_{\rm LO})(l)}$$

$$\times\left(F^{(l)}_{q_1\to P_0\otimes q_1}\left(x_{1\,m}, x_{2\,n}, \xi_F^2 Q^2{}_k\right) + F^{(l)}_{q_2\to P_0\otimes q_2}\left(x_{1\,m}, x_{2\,n}, \xi_F^2 Q^2{}_k\right)\right)\Bigg]\Bigg\},$$

where $F^{(l)}_{q_1\to P_0\otimes q_1}$ is calculated as $F^{(l)}$, but with q_1 replaced with $P_0\otimes q_1$(LO splitting function convoluted with PDF), and analogously for $F^{(l)}_{q_2\to P_0\otimes q_2}$.

APPLGRID applications.

Theoretical uncertainties:

- PDF uncertainty
- Scale uncertainty (Arbitrary simultaneous variation of renormalisation and factorisation scales a posteriori)
- Strong coupling uncertainty
- Can be calculated for any PDF and α_s in $\sim$ 10 *ms*
- A posteriori variation of centre-of-mass energy and fast evaluation of theoretical uncertainty in total cross section.

Allows rigorous inclusion of jet and electroweak cross sections in NLOQCD PDF fit.

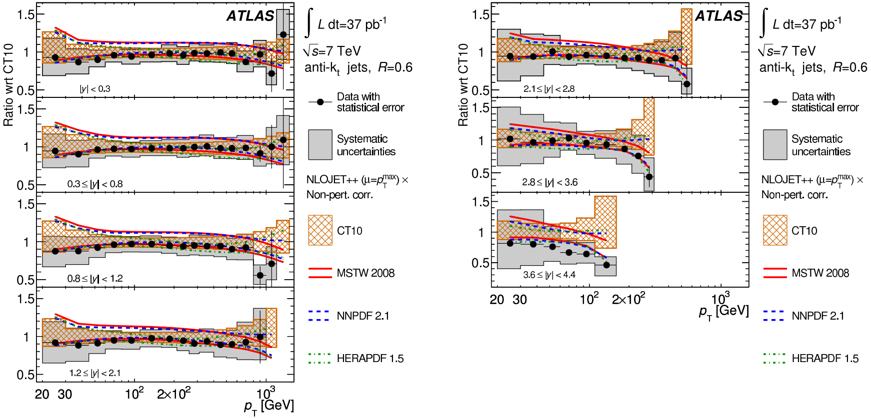
APPLGRID subprocesses for jet production

perturbative coefficients for jet production could be organised in seven subprocesses (calculated using NLOJET++)

$$
\begin{aligned}
\mathrm{gg}: \quad F^{(0)}(x_1, x_2; Q^2) &= G_1(x_1)G_2(x_2) \\
\mathrm{qg}: \quad F^{(1)}(x_1, x_2; Q^2) &= \left(Q_1(x_1) + \overline{Q}_1(x_1)\right) G_2(x_2) \\
\mathrm{gq}: \quad F^{(2)}(x_1, x_2; Q^2) &= G_1(x_1) \left(Q_2(x_2) + \overline{Q}_2(x_2)\right) \\
\mathrm{qq}': \quad F^{(3)}(x_1, x_2; Q^2) &= Q_1(x_1)Q_2(x_2) + \overline{Q}_1(x_1)\overline{Q}_2(x_2) - D(x_1, x_2) \\
\mathrm{qq}: \quad F^{(4)}(x_1, x_2; Q^2) &= D(x_1, x_2) \\
\mathrm{q\bar{q}}: \quad F^{(5)}(x_1, x_2; Q^2) &= \overline{D}(x_1, x_2) \\
\mathrm{q\bar{q}}': \quad F^{(6)}(x_1, x_2; Q^2) &= Q_1(x_1)\overline{Q}_2(x_2) + \overline{Q}_1(x_1)Q_2(x_2) - \overline{D}(x_1, x_2)
\end{aligned}
$$

$$
D(x_1, x_2) = \sum_{\substack{i=-6 \\ i\neq 0}}^{6} f_{i/H_1}(x_1, Q^2) f_{i/H_2}(x_2, Q^2), \quad \overline{D}(x_1, x_2) = \sum_{\substack{i=-6 \\ i\neq 0}}^{6} f_{i/H_1}(x_1, Q^2) f_{-i/H_2}(x_2, Q^2)
$$

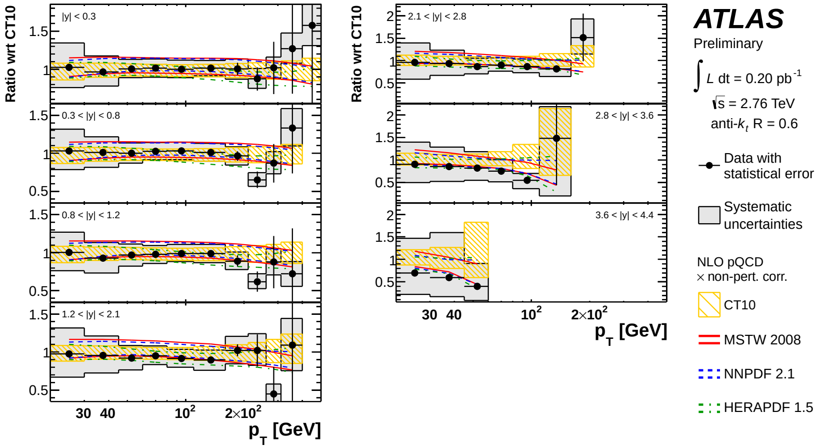
Inclusive jets: 7TeV collisions



Ratios of inclusive jet double-differential cross section to the theoretical prediction obtained using nlojet++ with the CT10 PDF set.

The ratios are shown as a function of jet p_T in different regions of $|y|$ for jets identified using the anti-kt algorithm with $R = 0.6$.

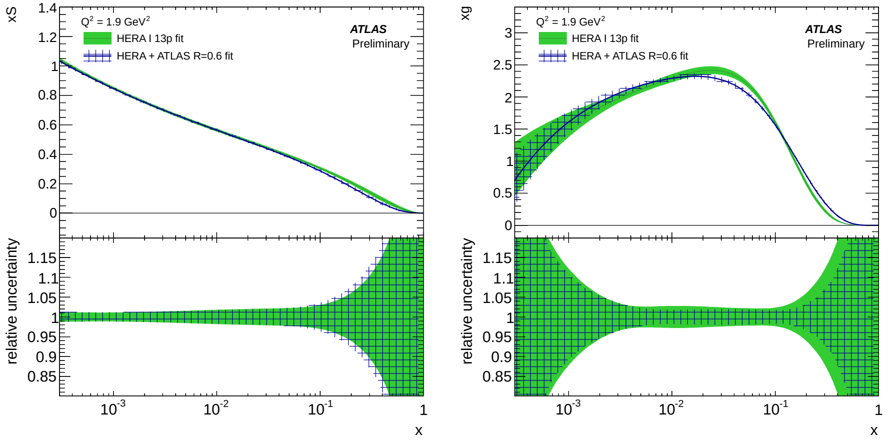
Inclusive jets: 2.76TeV collisions



Ratio of the measured inclusive double-differential jet cross section to the NLO pQCD prediction calculated with nlojet++ with the CT10 PDF set corrected for non-perturbative effects. The ratio is shown as a function of the jet p_{T} in bins of jet rapidity, for anti-kt jets with $R = 0.6$.

ATLAS jet data fit results

very good fit quality for both distance parameters



By including the ATLAS jet data, a harder gluon distribution and a softer sea quark distribution in the high Bjorken-x region are obtained with res pect to the fit of HERA-I data only.

The presented measurement is an interesting input for various PDF studies.

APPLGRID subprocesses for $W^{\pm}$ production

The weights for W^{+}-production can be organized in six possible initial state combinations (calculated using MCFM)

$$\bar{D}U: \quad F^{(0)}\left(x_1, x_2, Q^2\right) = \sum_{j=1,3,5} f_{-j/H_1}\left(x_1\right) \sum_{i=2,4,6} f_{i/H_2}\left(x_2\right) V_{ij}^2$$

$$U\bar{D}: \quad F^{(1)}\left(x_1, x_2, Q^2\right) = \sum_{i=2,4,6} f_{i/H_1}\left(x_1\right) \sum_{j=1,3,5} f_{-j/H_2}\left(x_2\right) V_{ij}^2$$

$$Ug: \quad F^{(3)}\left(x_1, x_2, Q^2\right) = \sum_{i=2,4,6} f_{i/H_1}\left(x_1\right) \left(V_{id}^2 + V_{is}^2 + V_{ib}^2\right) f_{0/H_2}\left(x_2\right)$$

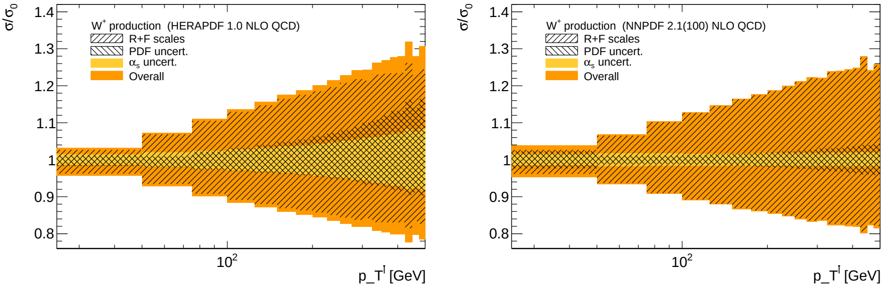
$$gU: \quad F^{(5)}\left(x_1, x_2, Q^2\right) = \sum_{i=2,4,6} f_{0/H_1}\left(x_1\right) \left(V_{id}^2 + V_{is}^2 + V_{ib}^2\right) f_{i/H_2}\left(x_2\right)$$

$$g\bar{D}: \quad F^{(4)}\left(x_1, x_2, Q^2\right) = \sum_{i=1,3,5} f_{0/H_1}\left(x_1\right) \left(V_{iu}^2 + V_{ic}^2 + V_{it}^2\right) f_{-i/H_2}\left(x_2\right)$$

$$\bar{D}g: \quad F^{(2)}\left(x_1, x_2, Q^2\right) = \sum_{i=1,3,5} f_{-i/H_1}\left(x_1\right) \left(V_{iu}^2 + V_{ic}^2 + V_{it}^2\right) f_{0/H_2}\left(x_2\right)$$

We separate $u\bar{d}$ from $\bar{d}u$ in order to get the right rapidity distribution for the electron, because of the chiral nature of the $W^{\pm}$ couplings

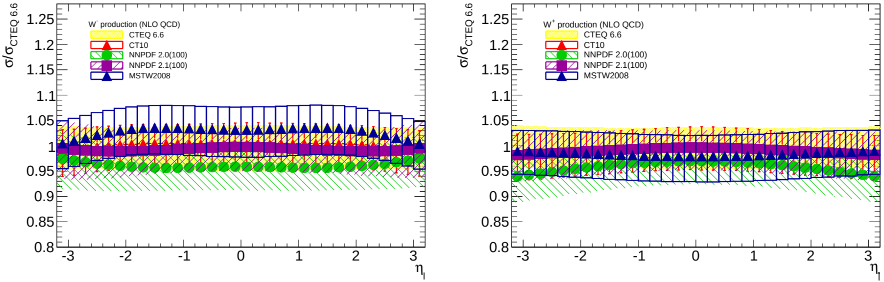
$W^{\pm}$ production theory uncertainties



positron p_T

- theoretical uncertainy decreases when adding more data (and more precise data) to pdf fits
- the scale uncertainty is the dominant one

$W^{\pm}$ production lepton rapidity. PDF comparison



electron positron

- different PDFs predict slightly different normalisation and shape

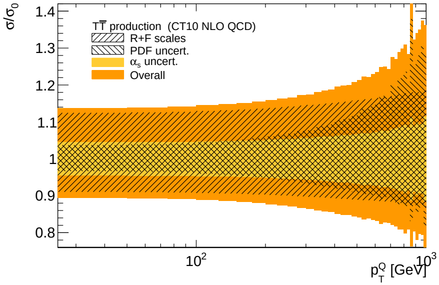
APPLGRID subprocesses for $Q\overline{Q}$ production

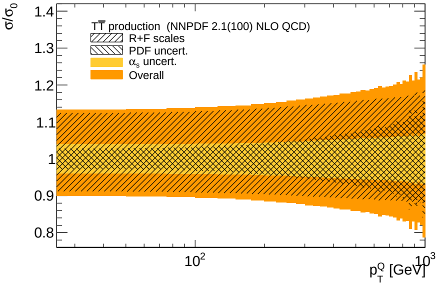
The weights for $Q\bar{Q}$-production can be organized in six possible initial state combinations (calculated using MCFM)

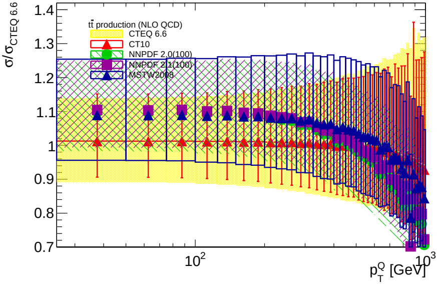
$$
\begin{aligned}
\mathrm{gg}: &\quad F^{(0)}(x_1, x_2; Q^2) = G_1(x_1)G_2(x_2) \\
\mathrm{qg}: &\quad F^{(1)}(x_1, x_2; Q^2) = Q_1(x_1)G_2(x_2) \\
\mathrm{gq}: &\quad F^{(2)}(x_1, x_2; Q^2) = G_1(x_1)Q_2(x_2) \\
\bar{\mathrm{q}}\mathrm{g}: &\quad F^{(3)}(x_1, x_2; Q^2) = \bar{Q}_1(x_1)G_2(x_2) \\
\mathrm{g}\bar{\mathrm{q}}: &\quad F^{(4)}(x_1, x_2; Q^2) = G_1(x_1)\bar{Q}_2(x_2) \\
\mathrm{q}\bar{\mathrm{q}}: &\quad F^{(5)}(x_1, x_2; Q^2) = D_{12}(x_1, x_2) \\
\bar{\mathrm{q}}\mathrm{q}: &\quad F^{(6)}(x_1, x_2; Q^2) = \bar{D}_{12}(x_1, x_2)
\end{aligned}
$$

number of quark flavours : $3(c\bar{c})$, $4(b\bar{b})$, $5(t\bar{t})$

$Q\overline{Q}$ production theory uncertainties



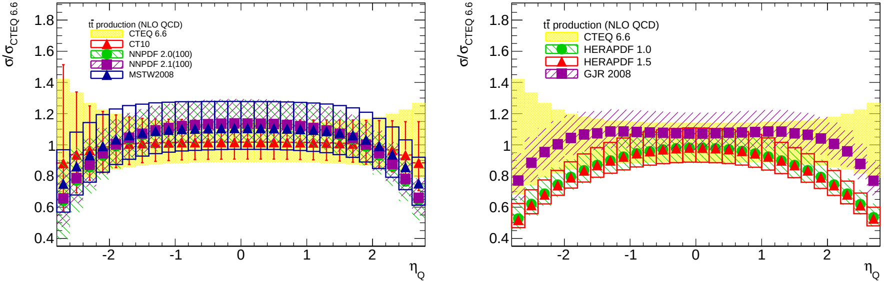




top p_T

- different shape and normalisation
- top differential measurements will provide constraints to PDFs

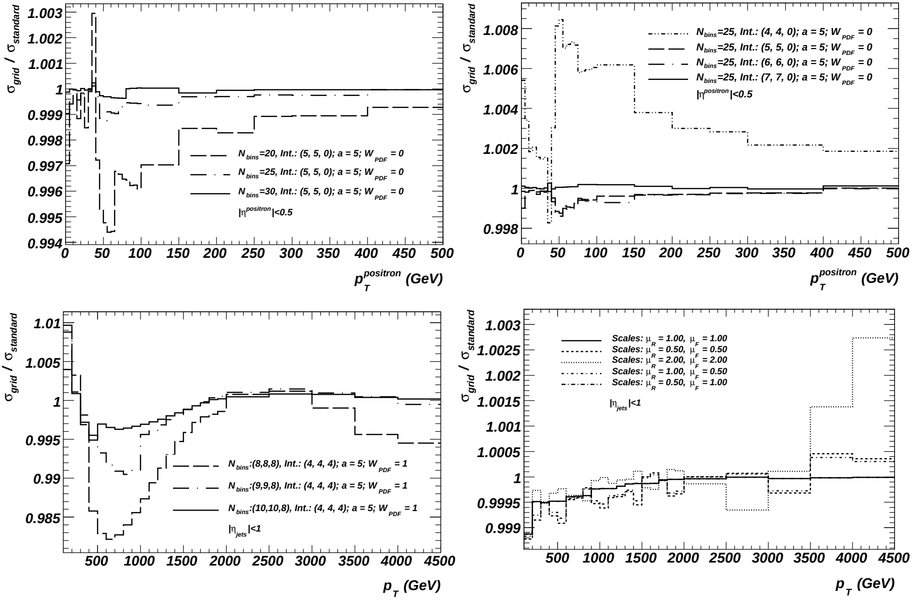
$Q\overline{Q}$ production PDF comparison



top rapidity

- different PDFs predict different shape

APPLGRID accuracy.



New physics : Quark contact interactions

Question : Could small deviations from SM predictions be absorbed by a N(N)LO QCD PDF fit?

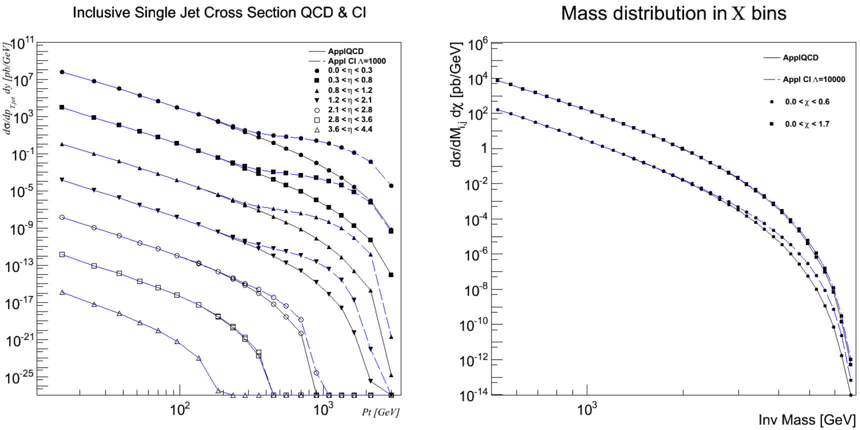
$$\frac{d\sigma}{d\mathcal{O}} = \frac{d\sigma_{QCD}}{d\mathcal{O}} + \eta\frac{\alpha_s}{\Lambda_{CI}^2}\frac{d\sigma_{CI}^{(1)}}{d\mathcal{O}} + \frac{1}{\Lambda_{CI}^4}\frac{d\sigma_{CI}^{(2)}}{d\mathcal{O}}$$

Phys.Lett. B253 (1991) 489-493

$\Lambda-$ CI scale; $\eta = \pm 1$ - interference with QCD

- generate phasespace using NLOJET++
- fill grids with CI ME
- convolute with PDF $+$ QCD coupling $+$ CI coupling within fit

Impact of CI on distributions



jet p_T dijet mass

Summary

Precision measurements test of QCD can improve knowledge of proton parton density functions and strong coupling constant and facilitate discoveries at LHC.

- APPLGrid is an open project, complete source code is available as HEPforge package:https://projects.hepforge.org/applgrid
- A posteriori evaluation of uncertainties from renormalisation and factorisation scale variations, strong coupling measurement and PDFs error sets in a very short time
- Allows rigorous inclusion of jet and electroweak cross sections in PDF fit.
- Other functionality, such as a posteriori $\sqrt{S}$ rescaling
- A list of QCD and electroweak processes can be studied
  - Jet production cross sections studied using NLOJET++
  - Electroweak observables included using MCFM
- New physics effects can be included in the fits

BACK-UP

APPLGRID interface to MCFM.

- MCFM : parton-level NLO QCD cross sections calculator for various femtobarn-level processes at hadron-hadron colliders.
  - V, $V + nJet$, $V + b\bar{b}$, VV, $Q\bar{Q}$,... ($\sim \mathcal{O}(300)$) http://mcfm.fnal.gov/
- Standard analysis :
  - at the end of each event MCFM provides the event record and the weight.
  - user routine (User/nplotter.f): calculates observable(s), applies cuts, fills weight
- APPLGRID is interfaced via common block
  - kinematics : $x_1, x_2, Q, ...$; dynamics :order, weights[]
  - C++ wrapper :
    - reads event record, calculates observable $\mathcal{O}$, fills the grid gridObject $\rightarrow$ fillMCFM($\mathcal{O}$);
    - fillMCFM(...) reads common block , performs subprocess decomposition, fills the weights

APPLGRID subprocesses for Z^0 production

We can introduce 12 sub-processes in Z production (calculated using MCFM)

$$
\begin{aligned}
U\bar{U}: &\quad F^{(0)}\left(x_1, x_2, Q^2\right) = U_{12}(x_1, x_2)\\
D\bar{D}: &\quad F^{(1)}\left(x_1, x_2, Q^2\right) = D_{12}(x_1, x_2)\\
\bar{U}U: &\quad F^{(2)}\left(x_1, x_2, Q^2\right) = U_{21}(x_1, x_2)\\
\bar{D}D: &\quad F^{(3)}\left(x_1, x_2, Q^2\right) = D_{21}(x_1, x_2)\\
gU: &\quad F^{(4)}\left(x_1, x_2, Q^2\right) = G_1(x_1)U_2(x_2)\\
g\bar{U}: &\quad F^{(5)}\left(x_1, x_2, Q^2\right) = G_1(x_1)\overline{U}_2(x_2)\\
gD: &\quad F^{(6)}\left(x_1, x_2, Q^2\right) = G_1(x_1)D_2(x_2)\\
g\bar{D}: &\quad F^{(7)}\left(x_1, x_2, Q^2\right) = G_1(x_1)\overline{D}_2(x_2)\\
Ug: &\quad F^{(8)}\left(x_1, x_2, Q^2\right) = U_1(x_1)G_2(x_2)\\
\bar{U}g: &\quad F^{(9)}\left(x_1, x_2, Q^2\right) = \overline{U}_1(x_1)G_2(x_2)\\
Dg: &\quad F^{(10)}\left(x_1, x_2, Q^2\right) = D_1(x_1)G_2(x_2)\\
\bar{D}g: &\quad F^{(11)}\left(x_1, x_2, Q^2\right) = \overline{D}_1(x_1)G_2(x_2)
\end{aligned}
$$

We separate $u\bar{u}$ from $\bar{u}u$ contributions to include γ/Z interference

APPLGRID subprocesses for Z^0 production II

Use is made of the generalised PDFs defined as:

$$U_H(x) = \sum_{i=2,4,6} f_{i/H}\left(x, Q^2\right), \qquad \overline{U}_H(x) = \sum_{i=2,4,6} f_{-i/H}\left(x, Q^2\right),$$

$$D_H(x) = \sum_{i=1,3,5} f_{i/H}\left(x, Q^2\right), \qquad \overline{D}_H(x) = \sum_{i=1,3,5} f_{-i/H}\left(x, Q^2\right),$$

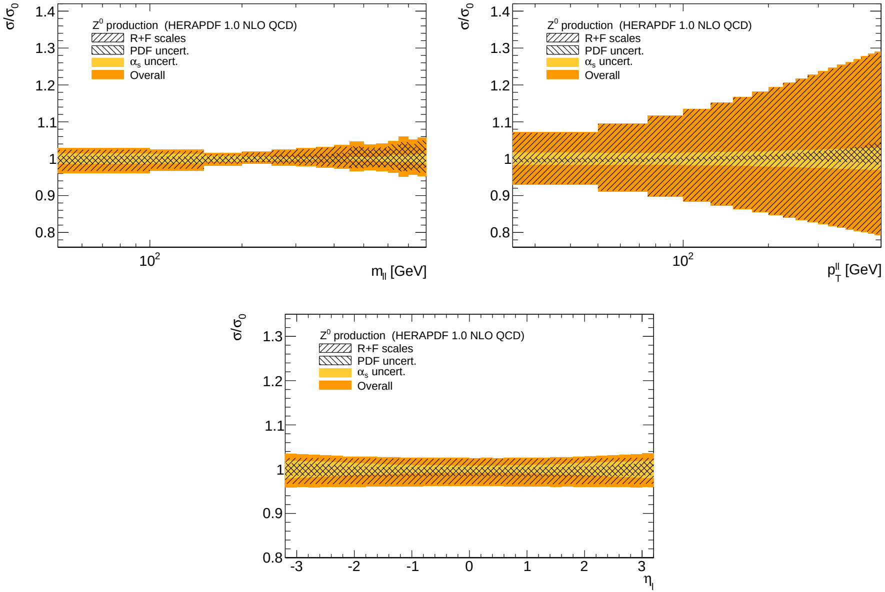
$$U_{12}(x_1, x_2) = \sum_{i=2,4,6} f_{i/H_1}\left(x_1, Q^2\right) f_{-i/H_2}\left(x_2, Q^2\right),$$

$$D_{12}(x_1, x_2) = \sum_{i=1,3,5} f_{i/H_1}\left(x_1, Q^2\right) f_{-i/H_2}\left(x_2, Q^2\right),$$

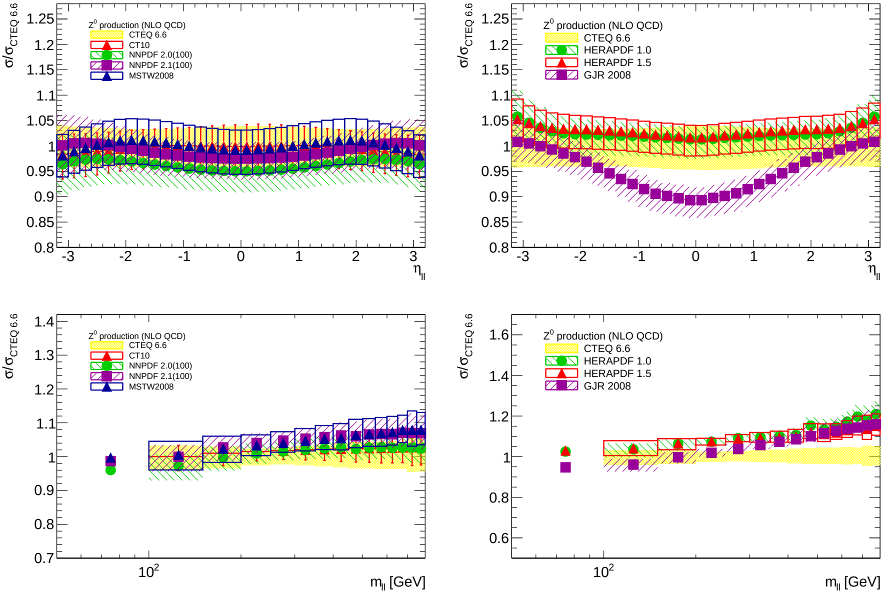
$$U_{21}(x_1, x_2) = \sum_{i=2,4,6} f_{-i/H_1}\left(x_1, Q^2\right) f_{i/H_2}\left(x_2, Q^2\right),$$

$$D_{21}(x_1, x_2) = \sum_{i=1,3,5} f_{-i/H_1}\left(x_1, Q^2\right) f_{i/H_2}\left(x_2, Q^2\right),$$

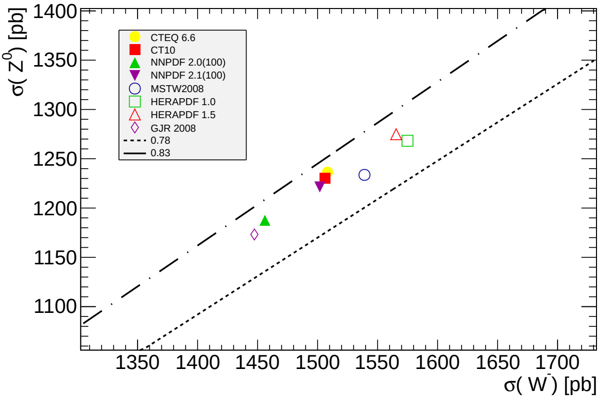
Z^0 production theory uncertainties



Z^0 production lepton rapidity. PDF comparison



Z^0 production Total cross section



different PDFs predict 10% different total cross section, but they all predict quite the same ratio.

NLOJET++

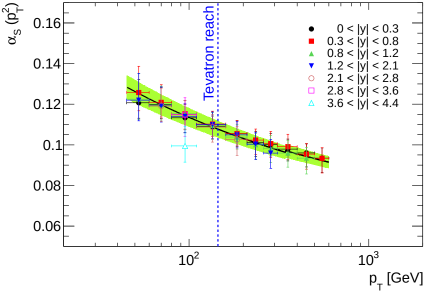
- input functions
  *void psinput(phasespace_hhc *ps, double& s)* : external phase space generator (if needed), energy [GeV] in C.M.S.

  void inputfunc(unsigned int& nj, unsigned int& nu, unsigned int& nd) : number of parton in final state at LO, number of UP(DOWN) quark flavors
- user class
  class UserHHC : public user1d_hhc {
  public:
  UserHHC(); ~UserHHC();
  void initfunc(unsigned int);
  void userfunc(const event_hhc&, const amplitude_hhc&);
  ...}
- *UserHHC* :: *userfunc*(...) (called every event)
  - *partons* $\xrightarrow{\textit{FastJet}}$ *jets*
  - event selection
  - *gridObject* → *fill*(...)

α_S determination

Eur.Phys.J. C72 (2012) 2041

- Input :
  - unfolded double-differential ATLAS inclusive jet cross section data at 7 TeV collisions.
  - NLO jet cross section corrected for NP effects
- Method :
  - The measured cross section in each (p_T, y) bin is mapped to α_S value.
  - All the experimental uncertainties of cross sections, together with their bin-to-bin correlations, are propagated to the determined α_S values, using pseudo-experiments (toys).
- Result : weighted average across all bins



$$\alpha_S(M_Z^2) = 0.1151 \pm 0.0001\,(\text{stat.}) \pm 0.0047\,(\text{exp. syst.}) \pm 0.0014\,(p_T\text{ range}) \pm 0.0060\,(\text{jet size})$$
$$^{+0.0044}_{-0.0011}\,(\text{scale})^{+0.0022}_{-0.0015}\,(\text{PDF choice}) \pm 0.0010\,(\text{PDF eig.})^{+0.0009}_{-0.0034}\,(\text{NP corrections}),$$