Using APPLGRID

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DESY

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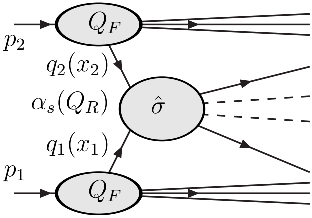
NLO QCD cross section



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

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

- 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

$\Longrightarrow$ we can split calculation into two parts

APPLGRID applications.

Calculation of theoretical uncertainties:

- PDF uncertainty
- Scale uncertainty (Arbitrary simultaneous variation of renormalisation and factorisation scales a posteriori)
- Strong coupling uncertainty
- Can be re-calculated for any PDF and/or α_s on-fly (in $\sim$ *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

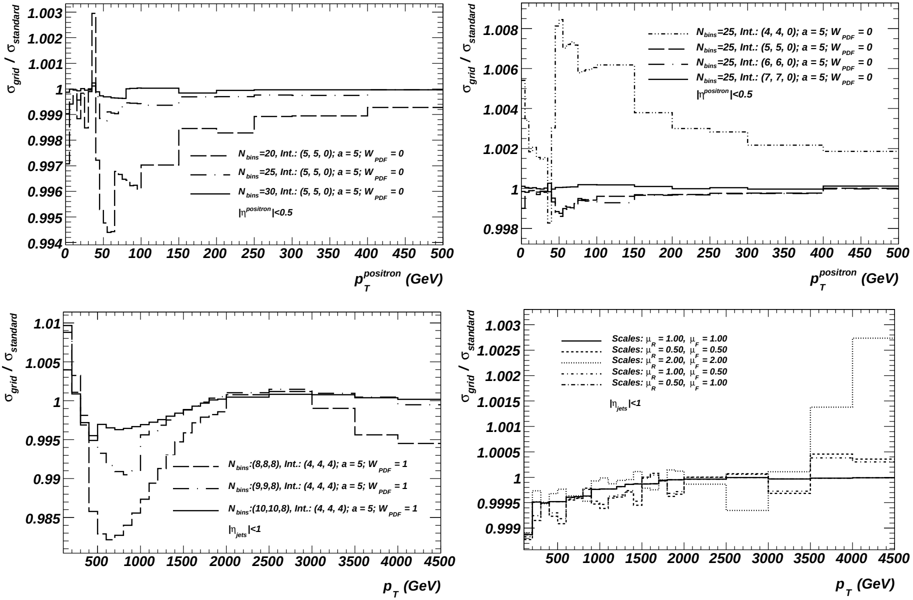
Practical issues. APPLGRID

- Define structure :
  observable, grid binning, grid interpolation
- Book a grid
  gridObject = new appl::grid(
  nObsBins,obsBins[],
  nQ2Bins, Q2Low, Q2High, interpolationOrderQ2,
  nXBins, xLow, xHigh, interpolationOrderX,
  processTag, lowestOrder, nLoops);
- Fill a grid
  event record $\Longrightarrow$ observable, scales, weights
  gridObject $\rightarrow$ fill(x_1, x_2, Q^2, $\mathcal{O}$, weight[], order);
- Convolute a grid
  select pdfSet, strong coupling, ...
  TH1D* h = gridObject $\rightarrow$ convolute(PDF, α_s , nLoops, μ_R, μ_F);
  std::vector$\langle$double$\rangle$ v = gridObject $\rightarrow$ vconvolute(PDF, α_s , nLoops, μ_R, μ_F);
  $(*)$ double d = gridObject $\rightarrow$ dconvolute(iBin, PDF, α_s , nLoops, μ_R, μ_F);

APPLGRID interface to MCFM.

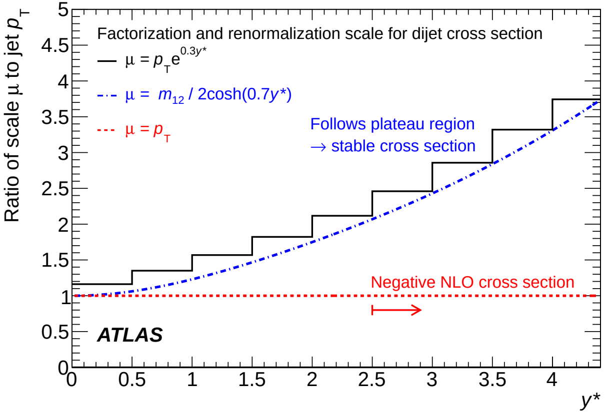
- MCFM : parton-level NLO QCD cross sections calculator for various femtobarn-level processes at hadron-hadron colliders.
  - V, $V + nJet$, $V + b\bar{b}$, VV, $Q\bar{Q}$,... ($\sim \mathcal{O}(300)$) http://mcfm.fnal.gov/
- Standard analysis :
  - at the end of each event MCFM provides the event record 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 accuracy.



New developments I

Functional change of scales : $\mu \to \mu(Q, \mathcal{O}, ...)$



The grid have to be regenerated, if the scale change requires additional variables not recorded.

New developments II

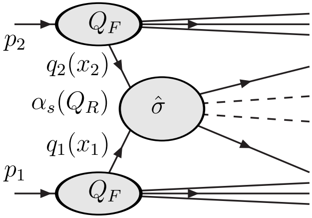
- The basic functionality for applying simple bin-by-bin corrections (additive and multiplicative) and global normalisation factor.
  - Convolution could be done with/without corrections
  - User can read in an external correction.
- Grids include additional documentation with full description of observable, like secondary binning, cuts, dimension, reference to publication, etc.
- We have new web site... (with grids for recent ATLAS jet measurements)
- We are starting to work on interface to DYNNLO

Summary

- APPLGrid is an open project, complete source code is available as HEPforge package:https://projects.hepforge.org/applgrid
- Rigorous inclusion of jet and electroweak cross sections in PDF fit. A list of QCD and electroweak processes can be studied
  - Jet production cross sections studied using NLOJET++ (up to 3 jets @NLO)
  - Electroweak observables included using MCFM ($W^{\pm}$, Z^{0}, $Q\bar{Q}$ are already implemented, the rest is straight forward)
- A posteriori evaluation of uncertainties from renormalisation and factorisation scale variations, strong coupling measurement and PDFs error sets in a very short time
- Other functionality, such as a posteriori $\sqrt{S}$ rescaling

BACK-UP

NLO QCD cross section



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- Coupling and parton density functions are non-perturbative inputs to calculation (extracted from data)
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$\Longrightarrow$ 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 .

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

  - binning (+ interpolation)
  - sub-processes $13 \times 13 \rightarrow \mathcal{L}$

- Step 2 ($\sim$ 10–100 ms): Convolute grid with PDF's .

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

  - integral $\rightarrow$ sum
  - any coupling, pdf

Details of the method I

Binning

- user defined number of bins N_x and N_{Q^2} in x and Q^2
- variable transformation $(x, Q^2) \to (y, \tau)$ 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.
  - $\Lambda \sim \Lambda_{\mathrm{QCD}}$, is user defined.
- 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 :

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

Details of method. 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 renormalization μ_R and factorization 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,

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

Details of method Scale dependence II

Then for arbitrary ξ_R and ξ_F we may write:

$$\frac{d\sigma}{dX}(\xi_R, \xi_F) = \sum_{l=0}^{L} \sum_{m} \sum_{n} \sum_{k} \left\{ \left(\frac{\alpha_s\left(\xi_R^2 {Q^2}_k\right)}{2\pi} \right)^{p_{\rm LO}} \right.$$

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

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

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

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

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 subprocesses for $W^{\pm}$ production

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

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

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

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

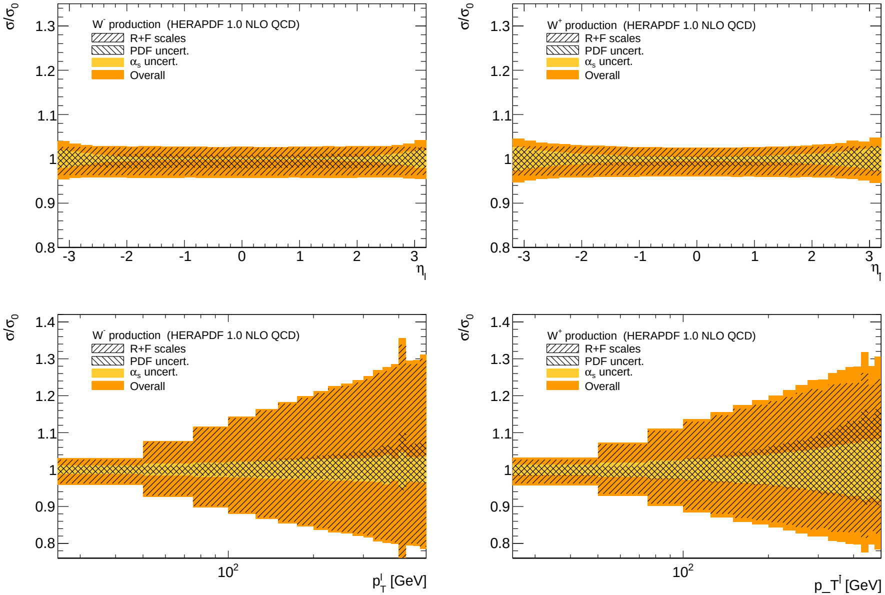
$$gU: \quad F^{(5)}\left(x_1, x_2, Q^2\right) = \sum_{i=2,4,6} f_{0/H_1}\left(x_1\right) \left(V_{id}^2 + V_{is}^2 + V_{ib}^2\right) f_{i/H_2}\left(x_2\right)$$

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

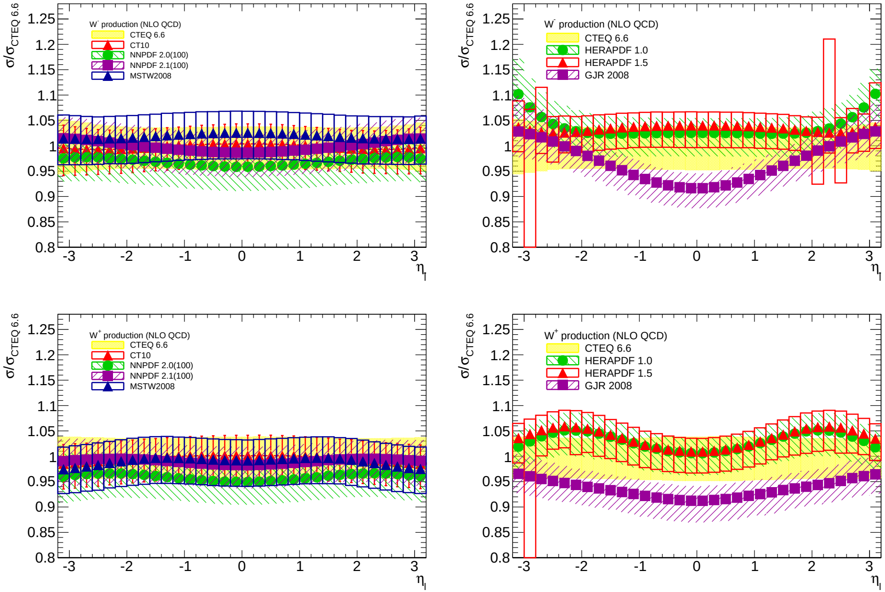
$$\bar{D}g: \quad F^{(2)}\left(x_1, x_2, Q^2\right) = \sum_{i=1,3,5} f_{-i/H_1}\left(x_1\right) \left(V_{iu}^2 + V_{ic}^2 + V_{it}^2\right) f_{0/H_2}\left(x_2\right)$$

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

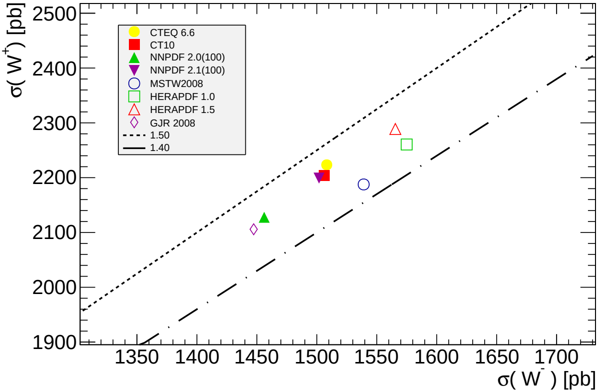
$W^{\pm}$ production theory uncertainties



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



$W^{\pm}$ production Total cross section



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

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:

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

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

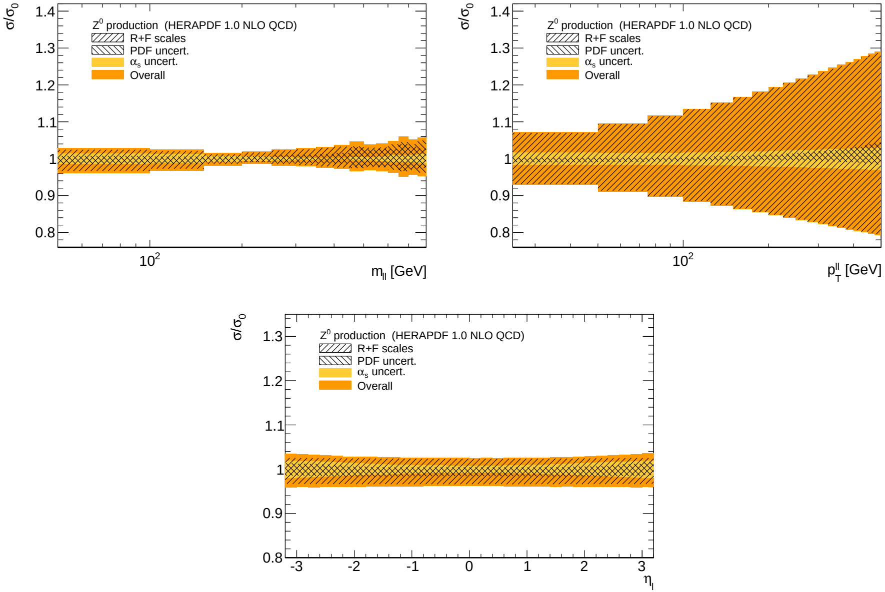
$$U_{12}(x_1, x_2) = \sum_{i=2,4,6} f_{i/H_1}\left(x_1, Q^2\right) f_{-i/H_2}\left(x_2, Q^2\right),$$

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

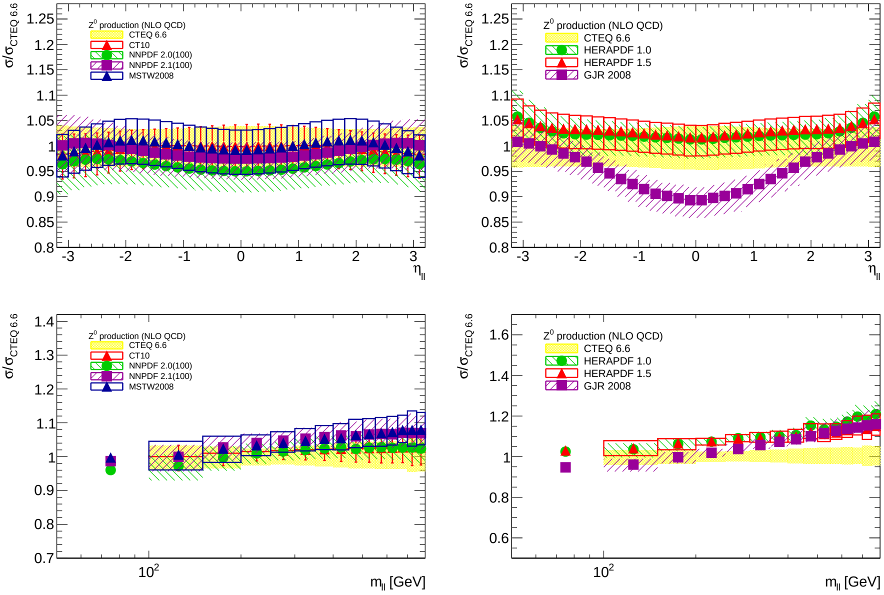
$$U_{21}(x_1, x_2) = \sum_{i=2,4,6} f_{-i/H_1}\left(x_1, Q^2\right) f_{i/H_2}\left(x_2, Q^2\right),$$

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

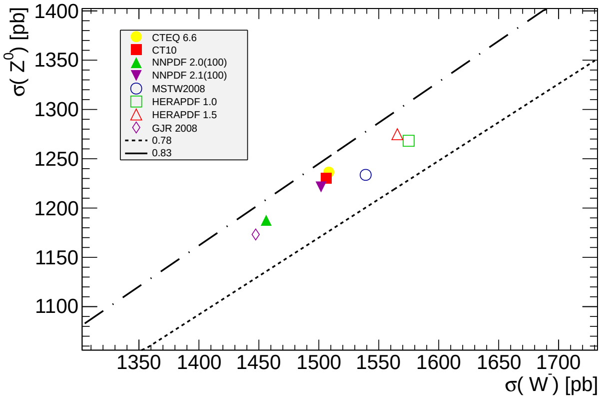
Z^0 production theory uncertainties



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.

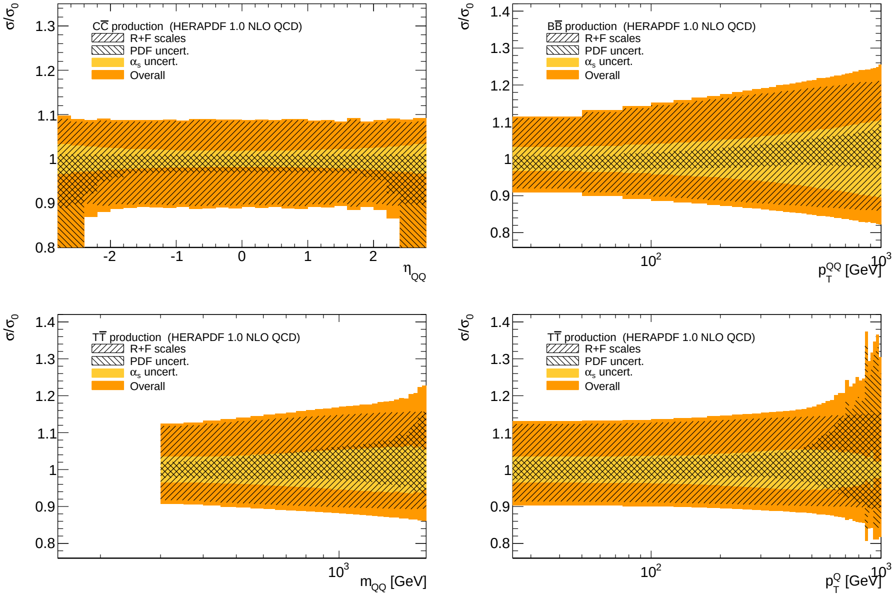
APPLGRID subprocesses for $Q\overline{Q}$ production

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

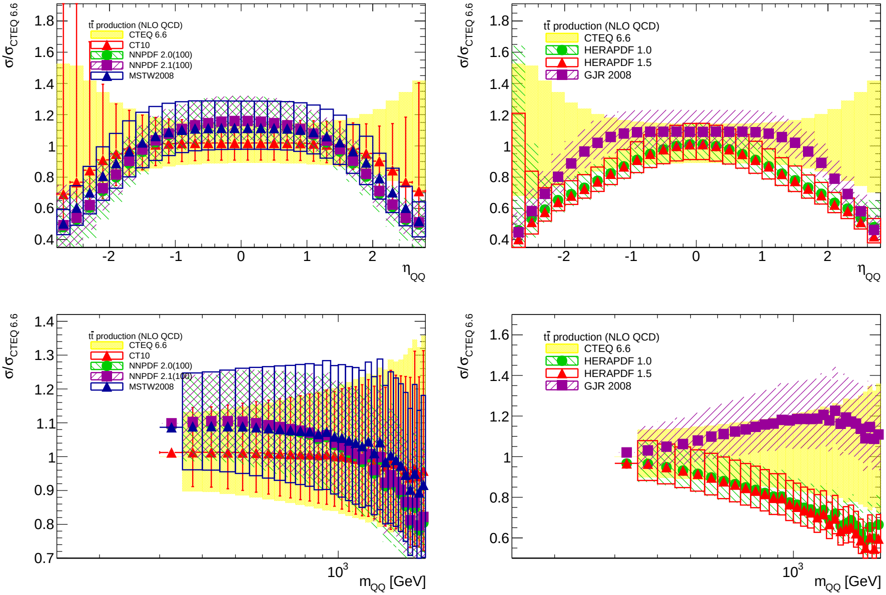
$$
\begin{aligned}
\mathrm{gg}: &\quad F^{(0)}(x_1, x_2; Q^2) = G_1(x_1)G_2(x_2) \\
\mathrm{qg}: &\quad F^{(1)}(x_1, x_2; Q^2) = Q_1(x_1)G_2(x_2) \\
\mathrm{gq}: &\quad F^{(2)}(x_1, x_2; Q^2) = G_1(x_1)Q_2(x_2) \\
\bar{\mathrm{q}}\mathrm{g}: &\quad F^{(3)}(x_1, x_2; Q^2) = \bar{Q}_1(x_1)G_2(x_2) \\
\mathrm{g}\bar{\mathrm{q}}: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

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

$Q\overline{Q}$ production theory uncertainties



$Q\overline{Q}$ production PDF comparison



$Q\overline{Q}$ production. 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*(. . .)