CTEQ NNLO PDFs, heavy flavors, and LHC data

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Outline

1. CT10 NNLO and CT12 NNLO parton distribution functions

2. A formalism for massive quarks in the CT10 fit at two-loop accuracy (S-ACOT-χ)

3. Benchmarking of QCD computations in PDF fits

4. LHC data in the CT12 global analysis

Two sets of CT NNLO error PDFs
1. CT10 NNLO eigenvector set

Available at http://hep.pa.msu.edu/cteq/public/ct10_2012.html**; is being submitted to LHAPDF; main focus of this talk**

Complements the CT10/CT10W NLO PDF sets *(Lai et al., PRD82, 074024 (2010))*

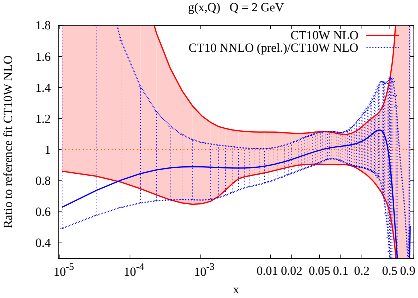
- **Includes only "pre-LHC" CT10 data.** Can be used to predict LHC cross sections based on pre-LHC experimental inputs
- Same input parameters, functional forms for input PDFs as in the CT10 NLO PDFs
  - $\alpha_s(M_Z) = 0.118 \pm 0.002$, $m_c^{pole} = 1.3$ GeV, $m_b^{pole} = 4.75$ GeV
  - Simpler assumptions about the PDF flavor composition at $\mu_0 = m_c^{pole} = 1.3$ GeV, *e.g.*, $\bar{u}(x)/\bar{d}(x) \to 1$ as $x \to 0$

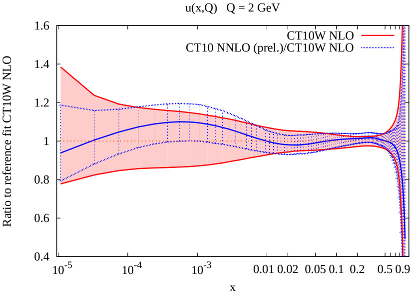
Two sets of CT NNLO error PDFs
1. CT12 NLO and NNLO eigenvector sets

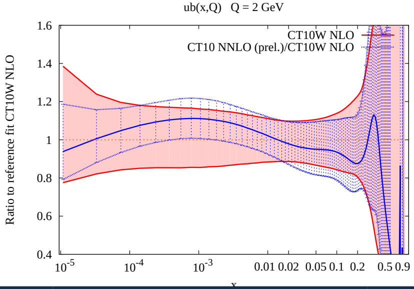
To be released within a few months

- Include LHC W and Z rapidity data, ATLAS and CMS jet data, HERA'2011 F_L data
- Updated α_s, m_c, m_b values
- Flexible $\bar{d}/\bar{u}$ ratio at $x \to 1$, updated $(s+\bar{s})/(\bar{u}+\bar{d})$ at $x \lesssim 10^{-2}$
    - Constrained by the LHC W/Z rapidity distributions

CT10 NNLO error PDFs (compared to CT10W NLO)







CT10 PDF sets: the naming conventions

- **Two NLO PDF sets**, without/with Tevatron Run-2 data on W charge asymmetry A_ℓ

CT10 NLO does not include
CT10W NLO includes
4 $p_{T\ell}$ bins of D0 Run-2 A_ℓ data

$\Rightarrow$ CT10 and CT10W sets differ mainly in the behavior of $d(x,Q)/u(x,Q)$ at $x > 0.1$

- **One NNLO PDF set:** only 2 inclusive $p_{T\ell}$ bins of D0 Run-2 A_ℓ data are included that have smallest theory uncertainties

- **The NNLO set is a counterpart of both CT10 NLO and CT10W NLO. It uses only a part of the A_ℓ data sample that distinguishes between CT10 NLO and CT10W NLO.**

Striving for NNLO accuracy in the PDFs

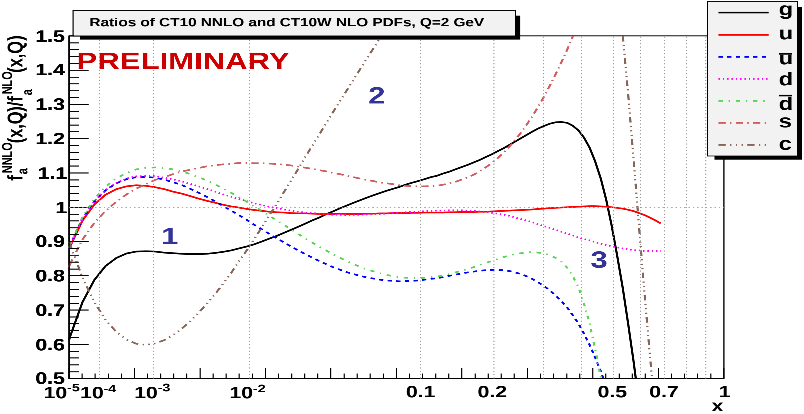
- So far, only "partial NNLO" global fits exist. For some fitted processes (inclusive jet production, CC DIS with $m_q \neq 0$), QCD contributions are known only to NLO. NLO EW contributions, power corrections, other systematic errors may be comparable to NNLO QCD effects.

- CT10 "NNLO" PDFs underwent validation studies for about one year. We identified several types of uncertainties that compete with NNLO QCD contributions.

- CT10 NNLO and NLO PDFs produce about the same $\chi^2/N_{pt} \approx 1.05 - 1.10$ for $N_{pt} = 2700$ data points

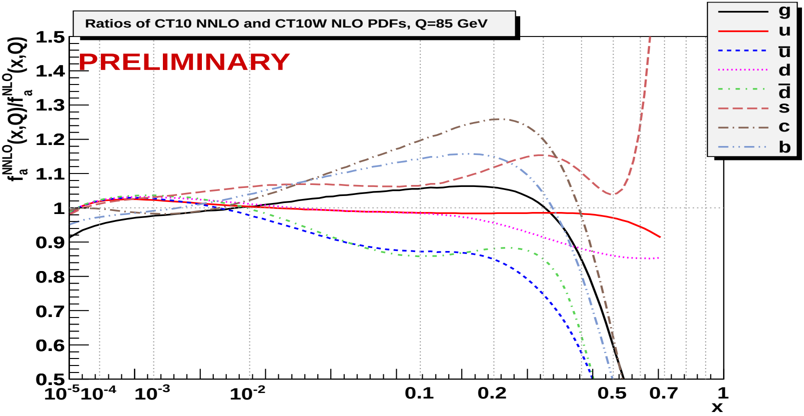
- Shapes of the NNLO PDFs have noticeably evolved compared to NLO as a result of $\mathcal{O}(\alpha_s^2)$ contributions, updated electroweak contributions, revised statistical procedures

CT10 NNLO central PDFs, as ratios to NLO, Q=2 GeV



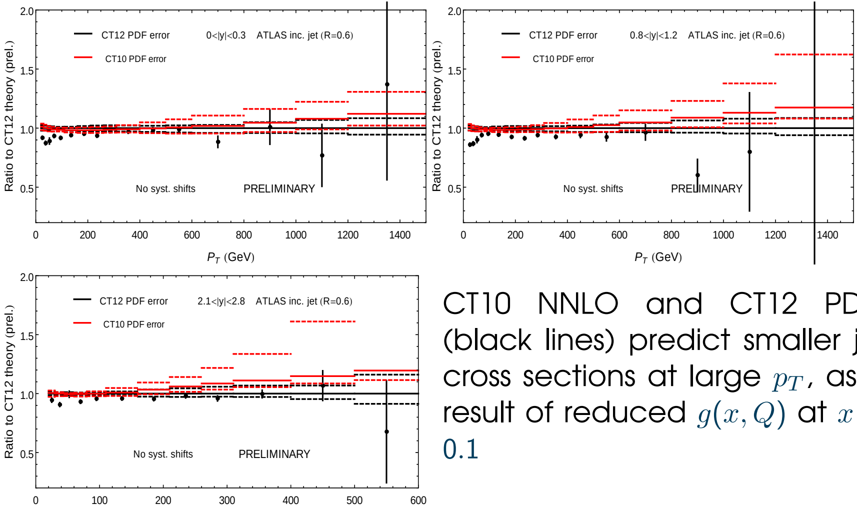
1. At $x < 10^{-2}$, $\mathcal{O}(\alpha_s^2)$ evolution suppresses $g(x,Q)$, increases $q(x,Q)$
2. $c(x,Q)$ and $b(x,Q)$ change as a result of the $\mathcal{O}(\alpha_s^2)$ GM VFN scheme
3. At $x > 0.1$, $g(x,Q)$ and $d(x,Q)$ are reduced by revised EW couplings, alternative treatment of correlated systematic errors, scale choices

CT10 NNLO central PDFs, as ratios to NLO, Q=85 GeV



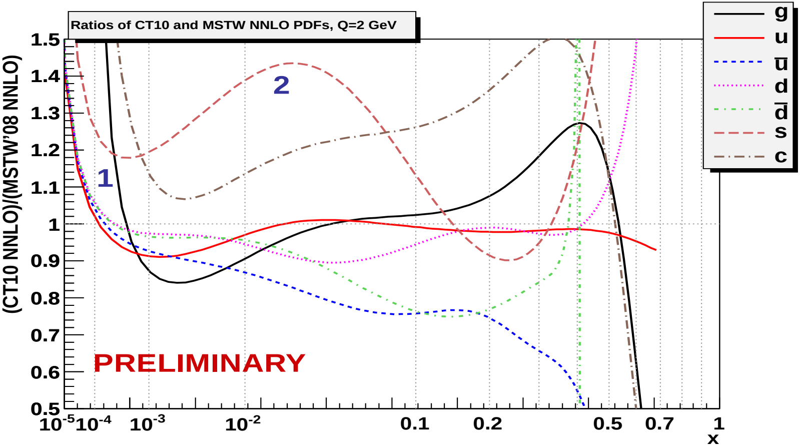
CT12 NLO predictions for LHC jet production

ATLAS single-inclusive jet production *(arXiv:1112.6297)*; FastNLO 2; R=0.6; $\chi^2/N_{d.o.f} = 0.72\,(0.98)$ for CT12 NLO (CT10 NLO)



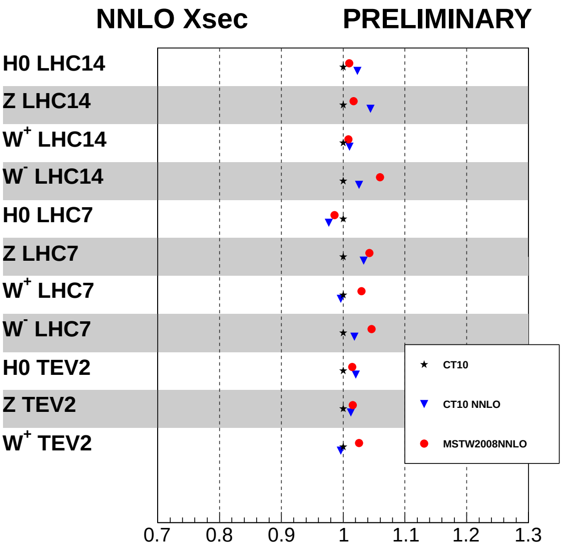
CT10 NNLO and CT12 PDFs (black lines) predict smaller jet cross sections at large p_T, as a result of reduced $g(x,Q)$ at $x > 0.1$

CT10 NNLO PDFs compared to MSTW NNLO



1. CT10 gluon and quarks are harder at $x \to 0$;
   $g(x, Q_0) > 0$ at $10^{-5} \leq x \leq 1$
2. The CT10 strange PDF is larger at $x \sim 10^{-3}$

Predictions for production of electroweak bosons



Details of the CT10 NNLO computation

- **NNLO hard-scattering contributions in DIS** (in the S-ACOT-χ mass scheme) and **vector boson production** (NNLO K factors from FEWZ for $d\sigma/dy$; NNLL/NLO+K from ResBos for W charge asymmetry)

- NNLO evolution for α_s and PDFs (HOPPET)
  - matching coefficients relating the PDFs in N_f and N_{f+1} schemes *(Smith, van Neerven, et al.)*

- Pole quark masses or $\overline{MS}$ quark masses as an input
  - CT10 NNLO: pole masses $m_c = 1.3$ GeV, $m_b = 4.75$ GeV

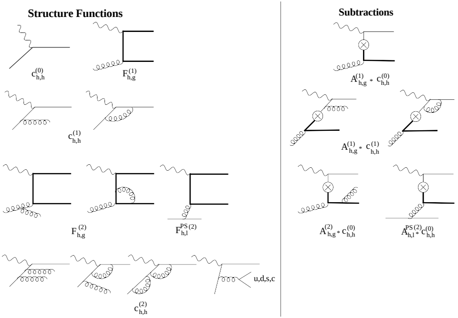
Neutral-current DIS in a general-mass scheme at NNLO

M. Guzzi, P.N., H.-L. Lai, C.-P. Yuan, arXiv:1108.5112 (hep-ph)

Objectives

- The CT10 fit computes c, b quark contributions to NC DIS in the S-ACOT-χ general-mass factorization scheme *(Aivasis, Collins, Olness, Tung, 1994; Collins, 1998; Kramer, Olness, Soper; Tung, Kretzer, Schmidt)*

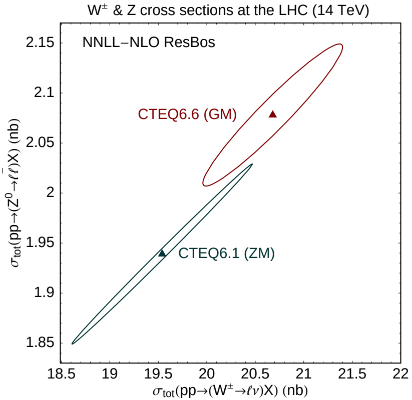
- We have realized this scheme at NNLO. We have also demonstrated how to derive this scheme (including kinematic rescaling of heavy-quark scattering terms at the mass threshold) from the QCD factorization theorem by Collins



NNLO scattering contributions

Massive quark contributions to neutral-current DIS...

...affect predictions for the LHC W and Z cross sections *(Tung et al., hep-ph/0611254)*



arXiv:0802.0007

Extensive recent work

Tung et al., hep-ph/0611254; Thorne, hep-ph/0601245; Tung, Thorne, arXiv:0809.0714; P.N., Tung, arXiv:0903.2667; Forte et al., arXiv:1001.2312; J. Rojo et al., arXiv:1003.1241;Alekhin, Moch, arXiv:1011.5790;...

Several heavy-quark factorization schemes

FFN, ACOT, BMSN, CSN, FONLL, TR'...

The NNLO realization of the S-ACOT-χ factorization scheme combines benefits of several approaches

Main features of the S-ACOT-χ scheme

- It is proved to all orders by the QCD factorization theorem for DIS *(Collins, 1998)*
- **Universal** PDFs
- It is relatively simple
  - One value of N_f (and one PDF set) in each Q range
  - sets $m_h = 0$ in ME with incoming $h = c$ or b
  - matching to FFN is **implemented at the level of the QCD factorization theorem**
- It reduces to the ZM $\overline{MS}$ scheme at $Q^2 \gg m_Q^2$, without additional renormalization
- It reduces to the FFN scheme at $Q^2 \approx m_Q^2$
  - has reduced dependence on tunable parameters at NNLO

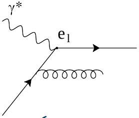
Components of inclusive $F_{2,L}(x,Q)$

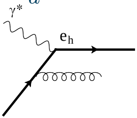
S-ACOT-χ NNLO expressions are reminiscent of the ZM scheme (e.g., in Moch, Vermaseren, Vogt, 2005), with all components available from literature

Components of inclusive $F_{2,L}(x,Q^2)$ are classified according to the quark couplings to the photon

$$F = \sum_{l=1}^{N_l} F_l + F_h \tag{1}$$

$$F_l = e_l^2 \sum_a \left[C_{l,a} \otimes f_{a/p}\right](x,Q), \quad F_h = e_h^2 \sum_a \left[C_{h,a} \otimes f_{a/p}\right](x,Q). \tag{2}$$



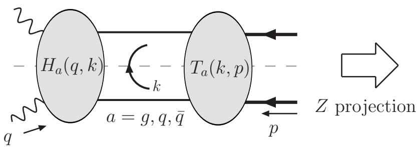


At $\mathcal{O}(\alpha_s^2)$:

$$F_h^{(2)} = e_h^2 \left\{ c_{h,h}^{NS,(2)} \otimes (f_{h/p} + f_{\bar{h}/p}) + C_{h,l}^{(2)} \otimes \Sigma + C_{h,g}^{(2)} \otimes f_{g/p} \right\}$$

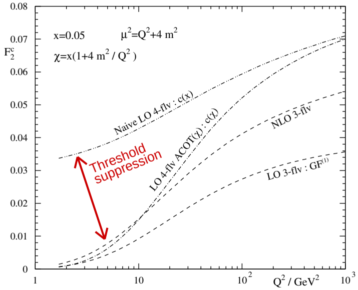
$$F_l^{(2)} = e_l^2 \left\{ C_{l,l}^{NS,(2)} \otimes (f_{l/p} + f_{\bar{l}/p}) + c^{PS,(2)} \otimes \Sigma + c_{l,g}^{(2)} \otimes f_{g/p} \right\}. \tag{3}$$

Rescaling to all orders of α_s and the factorization theorem

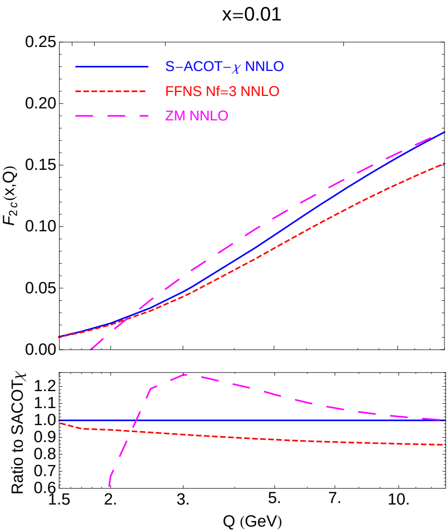


We show that a minor modification of the QCD factorization theorem *(Collins, 1998)...*

- enables suppression of charm production at $Q^2 \to m^2_{c,b}$ in all channels and at each α_s order without extra smoothness conditions or damping factors
- preserves universality of heavy-quark PDFs



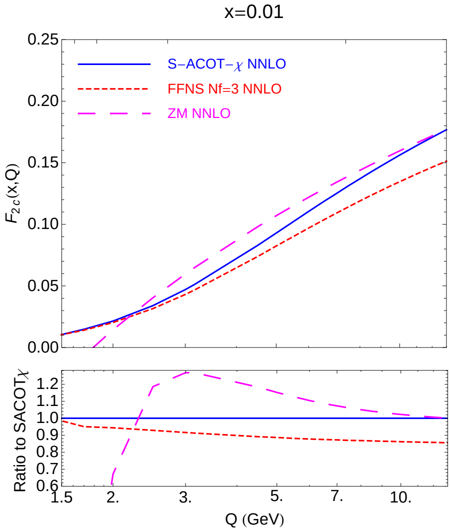
S-ACOT-χ scheme: merging FFN and ZM



ACOT reduces to FFNS at $Q \approx m_c$ and to ZM at $Q \gg m_c$

Les Houches toy PDFs, evolved at NNLO with threshold matching terms

S-ACOT-χ scheme: merging FFN and ZM



$\mathcal{O}(\alpha_s^2)$ flavor-creation contributions with $m_c \neq 0$ are included exactly *(based on the calculation by Riemersma, Smith, van Neerven, PL B347, 143 (1995))*

The implementation will be made available in HERA FITTER

A complementary calculation (a "hybrid mass scheme"; exact $\mathcal{O}(\alpha_s)$ massive ACOT terms + approximate $\mathcal{O}(\alpha_s^2)$ and $\mathcal{O}(\alpha_s^3)$ massive terms) has been published by *Stavreva, Olness, Schienbein, et al., arXiv:1203.0282*

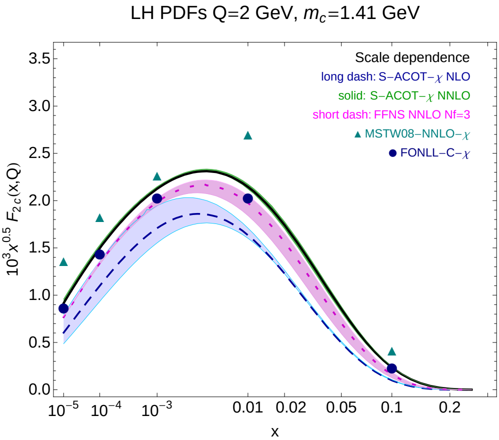
NNLO results for $F_2^{(c)}(x, Q^2)$

At NNLO and $Q \approx m_c$:

S-ACOT-$\chi\,(N_f = 4) \approx$ FFN $(N_f = 3)$
without tuning

- S-ACOT is numerically close to other NNLO schemes, especially the FONLL-C scheme

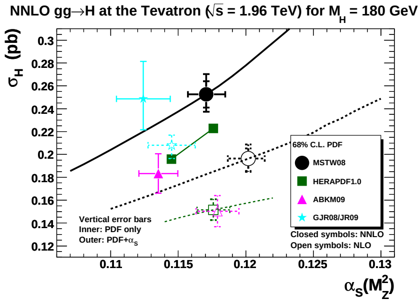
(Forte, Laenen, Nason, Rojo, arXiv:1001.2312).



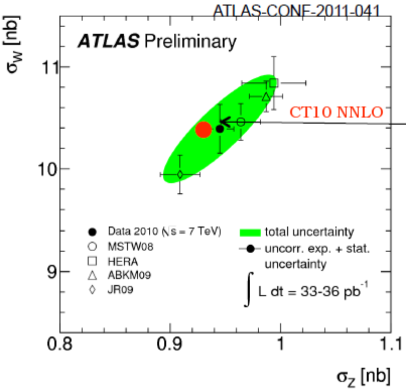
- The $\mathcal{O}(\alpha_s^2)$ S-ACOT-χ prediction is close to the FFN prediction at $Q \to m_c$ as a consequence of the kinematical rescaling introduced in the proof of factorization.

Control of uncertainties in NNLO PDF sets

Agreement between the existing NNLO PDF sets is not automatically better than at NLO. Differences are comparable to experimental errors



Thorne, Watt, arXiv:1106.5789



We performed several validation studies to identify the uncertainties that compete with NNLO corrections

Efforts to reduce differences between NNLO fits

1. Benchmarking comparisons of the fitting codes

1.1 Benchmarks for inclusive DIS cross sections
(with S. Alekhin, A. Glazov, A. Guffanti, J. Rojo)

$\Rightarrow$ importance of subleading/NLO EW effects

1.2. Benchmarks for NLO jet production calculations
(J. Gao, Z. Liang at SMU + J. Rojo representing ApplGrid)

$\Rightarrow$ effect on the large-x gluon PDF

2. Re-examination of correlated systematic uncertainties from both theory and experiment (in the backup slides)

1.1. Benchmarking of $\gamma^* Z$ interference of NC DIS cross sections

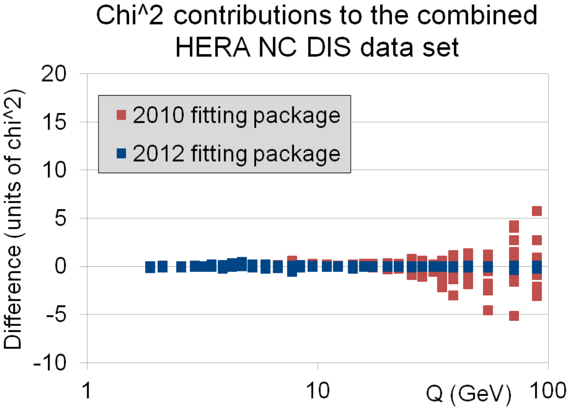
CTEQ implementation of the $\gamma^* Z$ interference terms in NC DIS is based on the helicity formalism *(Aivazis, Olness, Tung, 1994).* It shared definitions of EW couplings with vector boson production.

During the benchmarking, we modified the Z boson couplings to comply with the formulas for NC DIS in the combined HERA analysis *(arXiv:0911.0884).*

The revised CTEQ code was compared at ZM LO against another code *(A. Guffanti)*. Excellent agreement was reached.

This modification reduced $\bar{q}(x, Q), g(x, Q)$ at $x > 0.1$ in CT10 NNLO. Subleading EW contributions are relevant in this case.

1.1. Benchmarking of NC DIS cross sections



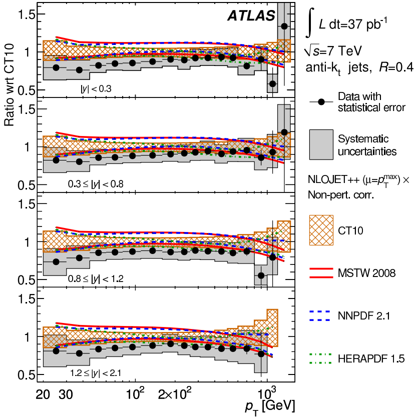
Point-by-point contributions to χ^2 for the combined HERA NC DIS set at ZM LO in the CTEQ code and alternative code (A. Guffanti). Some differences between two codes were observed at large Q, in the (x, Q) region where experimental errors also increase. Differences become practically zero after the benchmarking.

1.2 Benchmark comparison of NLO jet cross sections

J. Gao, Z. Liang, P. N., in 2011 Les Houches Proceedings, arXiv:1203.6803; in collaboration with D. E. Soper, H.-L. Lai, C.-P. Yuan

Benchmarking of NLO cross sections for inclusive jet and dijet production is needed to understand theory uncertainties at the LHC (including significant scale dependence at largest p_T^{jet})

It is also a preparation step toward the NNLO calculation for jet production



Modified EKS program *(publicly available)*

CTEQ fits have been using the EKS program, which realizes an NLO calculation for single-incl. jet and dijet production by S. D. **E**llis, Z. **K**unszt, and D. E. **S**oper *(PRL 69, 1496 (1992))*

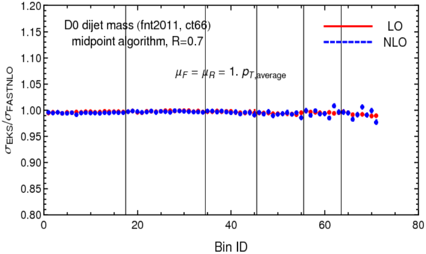
We modified the EKS code to calculate NLO jet cross sections more efficiently, with flexible input and output formats, and provide them in "almost differential" finely binned tables.

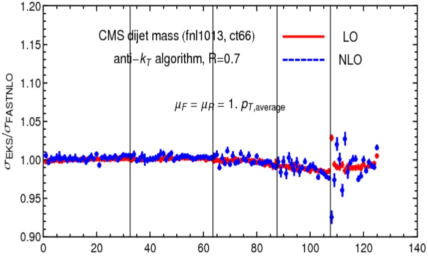
Other available programs include NLOJET++ *(Z. Nagy, PRL 88, 122003 (2002))* , FastNLO *(Kluge et. al., hep-ph/0609285)*, POWHEG *(Alioli et. al., JHEP 04081 (2011))*, ApplGrid *(EPJC66, 503 (2010))*

We identified specific conditions needed to reconcile MEKS and FastNLO outputs. For very specific settings of the jet algorithm, recombination scheme, jet trigger, QCD scale choices, MEKS and FastNLO show excellent agreement at most y^{jet}, p_T^{jet}, and M^{jj}.

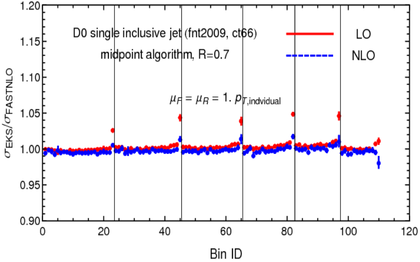
Comparison of MEKS and FastNLO 1.0

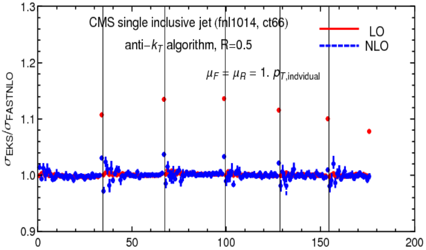
Dijet production: excellent agreement at both the Tevatron and LHC





Single-inclusive jet production: discrepancies of 3-10% exist at large p_T, possibly due to different definitions of the “jet p_T” used as the QCD scale.



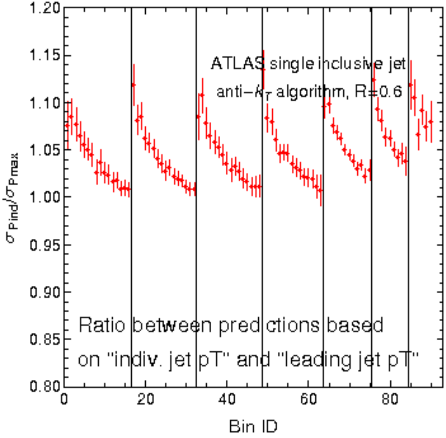


The choice of scale in jet production cross sections

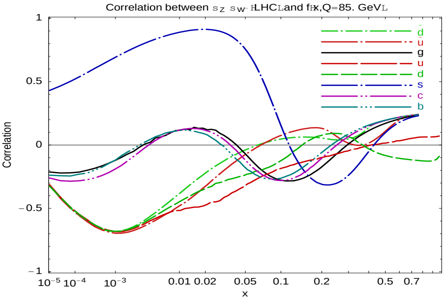
The *"jet p_T"* may refer to the *"p_T of the leading jet in an event"*, *"p_T of each jet in each p_T bin"*, *"average p_T in each p_T bin (FastNLO 1)"*, or *"p_T of the leading jet in each bin (ATLAS)"*. Differences resulting from these definitions are comparable to NNLO/PDF uncertainties.

CT10 NNLO/CT12 PDFs use $\mu_F = \mu_R = \langle p_T \rangle_{bin}$ and FastNLO 2 (implemented as an alternative to the K-factor lookup tables based on the MEKS calculation).

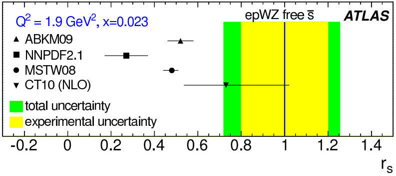
$\Rightarrow$ Softer gluon than in CT10 NLO



Strangeness in CT12 PDFs and LHC W/Z cross sections



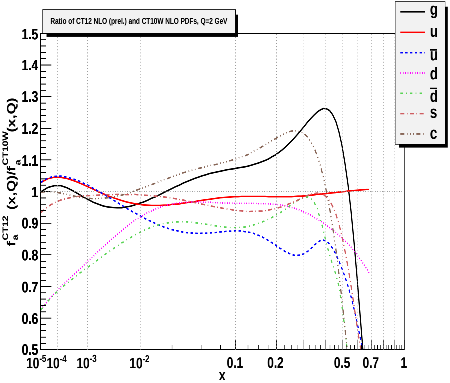
In 2008, our CTEQ6.6 PDF correlation analysis pointed out the sensitivity of ratios σ_W/σ_Z at the LHC to the strangeness PDF, with implications to EW precision measurements *(P.N., Lai, Cao, Huston, Pumplin, Tung, Yuan, PRD, 78 (2008) 013004)*.

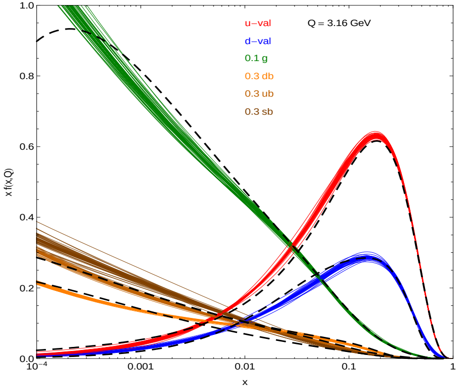


The ATLAS analysis (arXiv:1203.4051) of W and Z production suggests that $\bar{s}(x,Q)/\bar{d}(x,Q) = 1.00^{+0.25}_{-0.28}$ at $x = 0.023$ and $Q^2 = 1.9$ GeV^2

What is the impact of the new LHC W and Z data on the CT12 PDFs that will include them?

Small-x limits of $\bar{d}(x,Q)/\bar{u}(x,Q)$ and $\bar{s}(x,Q)/\bar{u}(x,Q)$ in the CT12 analysis (PRELIMINARY)





The CT12 analysis explores the possibility of $\lim_{x\to 0} \bar{d}/\bar{u} \neq 1$. Some "unbiased" CT12 candidate fits have $\bar{s}(x,Q)/\bar{u}(x,Q) > 1$ at $x < 10^{-3}$.

We would like to better understand the flavor decomposition at small x before releasing the CT12 PDFs.

Conclusions

- The CT10 NNLO PDF analysis (based on pre-LHC data only) is released. It is based on a new streamlined implementation of heavy-quark DIS contributions at two loops *(Guzzi et al., arXiv:1108.5112).*

- The CT12 NLO and NNLO analysis (in progress) will include latest LHC data on W, Z, and jet production. Possible impact on $SU(3)$ properties of quark sea at $x < 10^{-3}$.

- Several factors that are comparable to NNLO contributions (treatment of percentage corr. syst. errors, choices of scales, electroweak radiative contributions, ...) have been thoroughly examined in this analysis

- We use a specific choice to evaluate these factors in the CT12 (N)NLO fits. The uncertainty associated with this choice need to be examined in the future

Backup slides

2. Computation of correlated systematic errors

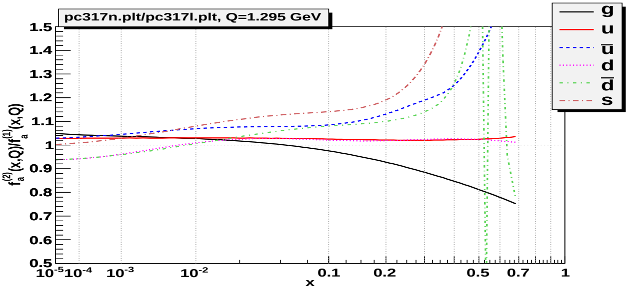
$$\chi^2 = \sum_{\{\text{exp.}\}} \left[\sum_{k=1}^{N_{pts}} \frac{1}{s_k^2} \left(D_k - T_k(\{a\}) - \sum_{\alpha=1}^{N_\lambda} \lambda_\alpha \beta_{k\alpha} \right)^2 + \sum_{\alpha=1}^{K_e} \lambda_\alpha^2 \right]$$

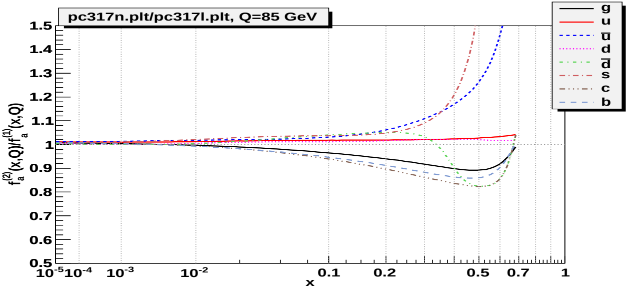
The experimental correlated systematic errors $\beta_{k\alpha}$ are often published as percentages. It can be taken to be a percentage of the theoretical prediction T_k ("truth") or the experimental datum D_k.

1. **Percentage of T_k:** results in smooth $\beta_{k\alpha}$:-); may depend on the theoretical model :-(
2. **Percentage of D_k:** $\beta_{k\alpha}$ is deduced from the measured data :-), but may not be smooth due to statistical fluctuations :-(

The methods are equivalent if T_k is close to D_k. In the actual CTXX fits to the Tevatron Run-2 jet data, **method 1** (used in pre-2012 CTEQ fits) results in a harder gluon at $x > 0.1$ than **in method 2**. We use **method 2** in the latest NNLO fits.

2.2. Impact on the best fit NLO PDFs





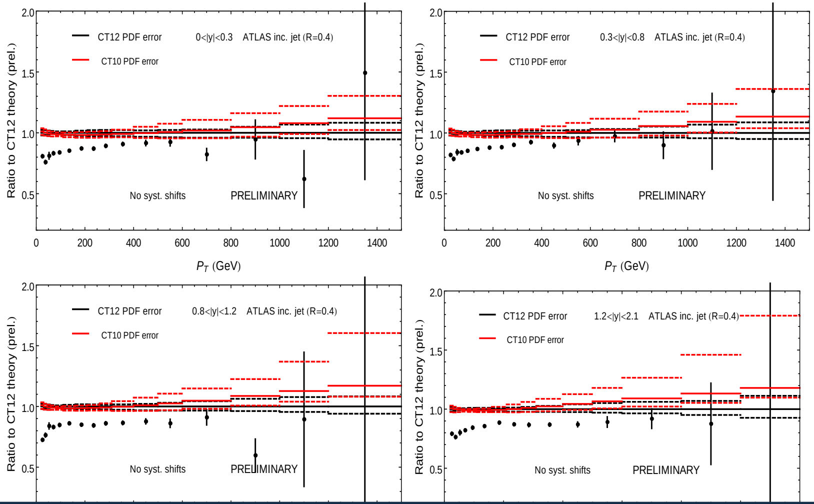
pc317l: CT12 NLO candidate obtained with method 1

pc317n: CT12 NLO candidate obtained with method 2

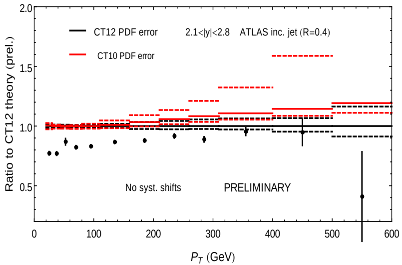
Notice changes in $u(x,Q)$, $d(x,Q)$, $g(x,Q)$

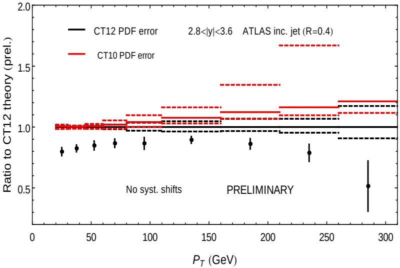
CT12 predictions for ATLAS jet production (2)

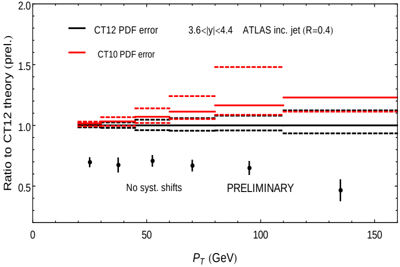
ATLAS single-inclusive jet production *(arXiv:1112.6297)*; FastNLO 2; R=0.4; $\chi^2/N_{d.o.f} = 0.76\,(0.95)$ for CT12 NLO (CT10 NLO)

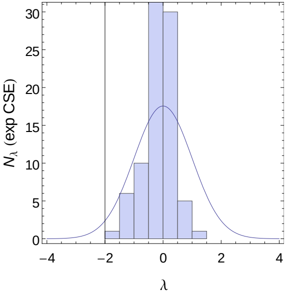


CT12 predictions for ATLAS jet production (3)









Factorization scale in NLO jet cross sections

NLO jet cross sections depend significantly on renorm. and fact. scales, μ_F and μ_R

CT10 fit assumed the default scale $\mu_F^0 = \mu_R^0 = p_T/2$; other groups and experimentalists often use $\mu_F^0 = \mu_R^0 = p_T$

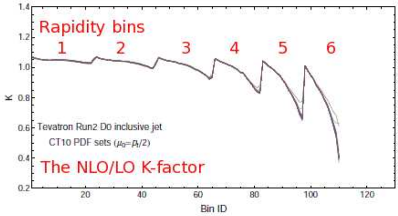
Trade-offs between the scale choices (see the next slide)

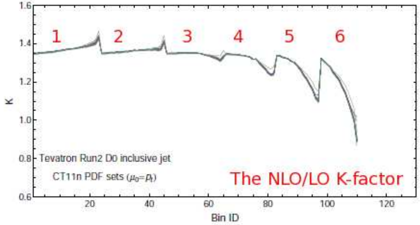
- $\mu_{F,R} = p_T/2$: $K \approx 1$ at small y_{jet}, large scale dependence at large y_{jet}
- $\mu_{F,R} = p_T$: $K \approx 1.4$ at small y_{jet}, smaller scale dependence at large y_{jet}

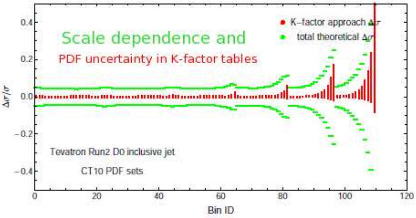
CT10 NNLO will provide a PDF set for $\mu_{F,R} = p_T$

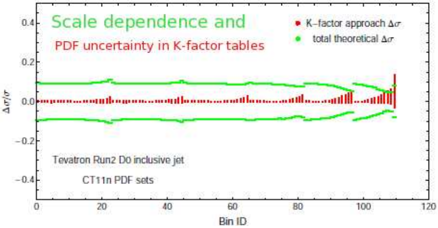
NLO corrections for $\mu^0_{F,R} = p_T/2$ (left) and p_T (right)

Jun Gao, 2011









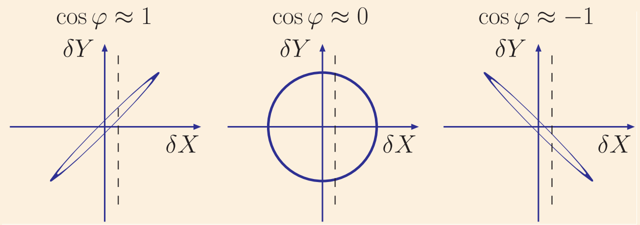
Scale dependence (green) corresponds to variations $1/2 \leq \mu_{F,R}/\mu^0_{F,R} \leq 2$. Red bands reflect the PDF uncertainty in the lookup tables for the NLO K-factors.

But which PDFs do the jet data exactly constrain?

Compute the PDF correlation cosine *(hep-ph/0101032; arXiv:0802.0007)*,

$$\cos\varphi \equiv \frac{1}{4\Delta X\,\Delta Y}\sum_{i=1}^{N_{PDF\,params}}\left(X_i^{(+)}-X_i^{(-)}\right)\left(Y_i^{(+)}-Y_i^{(-)}\right)$$

to establish which PDFs $X(x,Q)$ contribute most of the PDF uncertainty in the observable Y

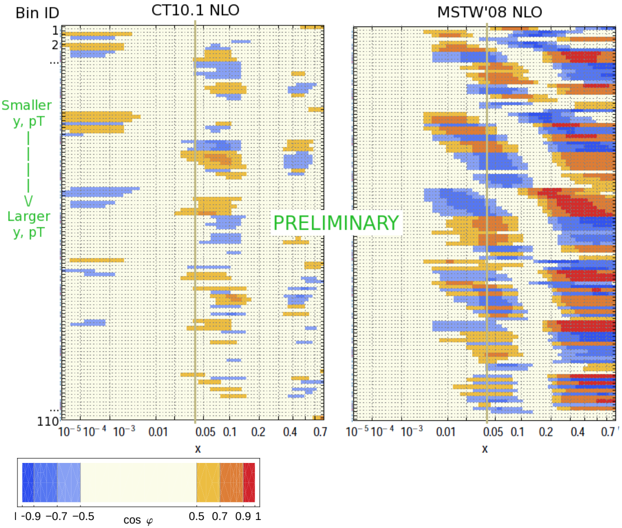


$\cos\varphi \approx \pm 1$: Measurement of Y imposes tight constraints on X

$\cos\varphi \approx 0$: Measurement of Y imposes loose constraints on X

Correlations between D0 Run-2 inc. jet data and gluon PDF

Z. Liang, P. Nadolsky, in 2011 Les Houches Proceedings



Correlation between $g(x, Q = 3.163$ GeV) and χ_i^2 in jet p_T bins (with syst. shifts)...

...is more pronounced for the MSTW'08 sets (right) than for CT10 sets (left)