



*REF2016 - November - Antwerp 2016, Belgium*

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# TMDs in xFitter

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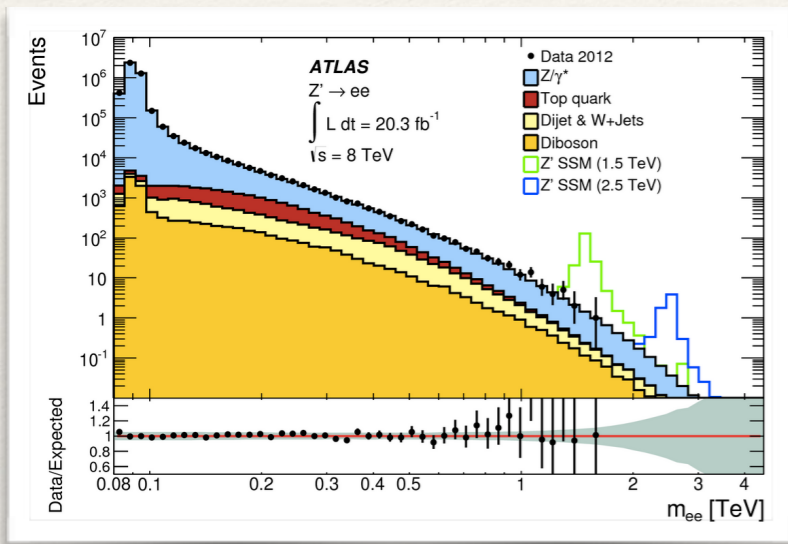
# Search for new Physics

direct searches  
for new physics

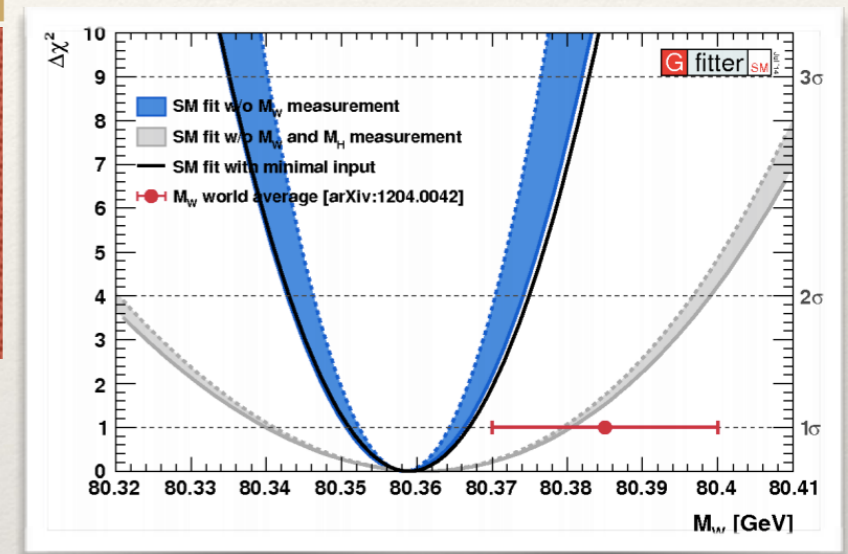
indirect searches via  
consistency test of SM

control of QCD background  
and SM parameters

Interpretation of any cross section  
measurement which involves  
hadron in the initial state relies on  
factorisation concept:



[arXiv:1410.6810v2]



Gfitter

$$\underbrace{\sigma(x, Q^2)}_{\text{hadronic } x\text{-sec.}} = \sum_{a,b} \int_0^1 dx_1 dx_2 \underbrace{f_a(x_1 Q^2) f_b(x_2 Q^2)}_{\text{PDFs}} \times \underbrace{\hat{\sigma}(x_1, x_2, Q^2)}_{\text{partonic } x\text{-sec.}}$$

taken from data      calculable

Improvement of PDFs precision demands high precision theory & experimental measurements

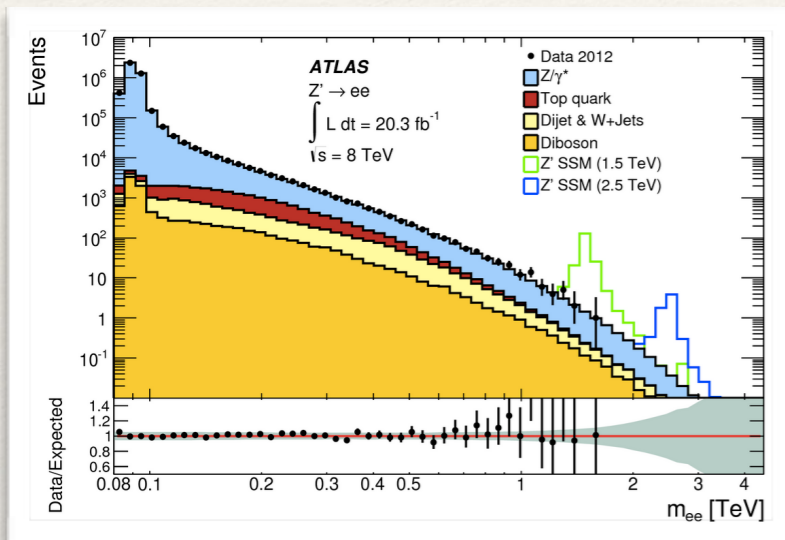
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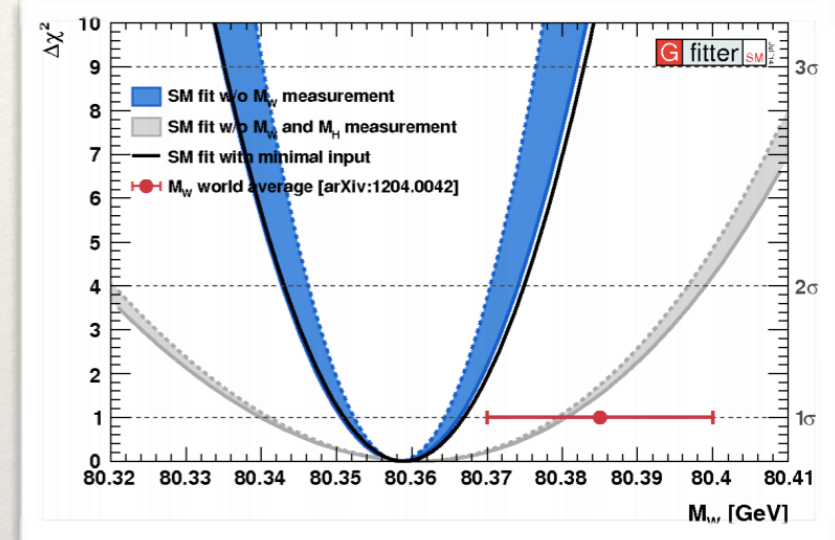
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taken from data

calculable

Further dimension of hadrons:  
PDFs dependent on kT

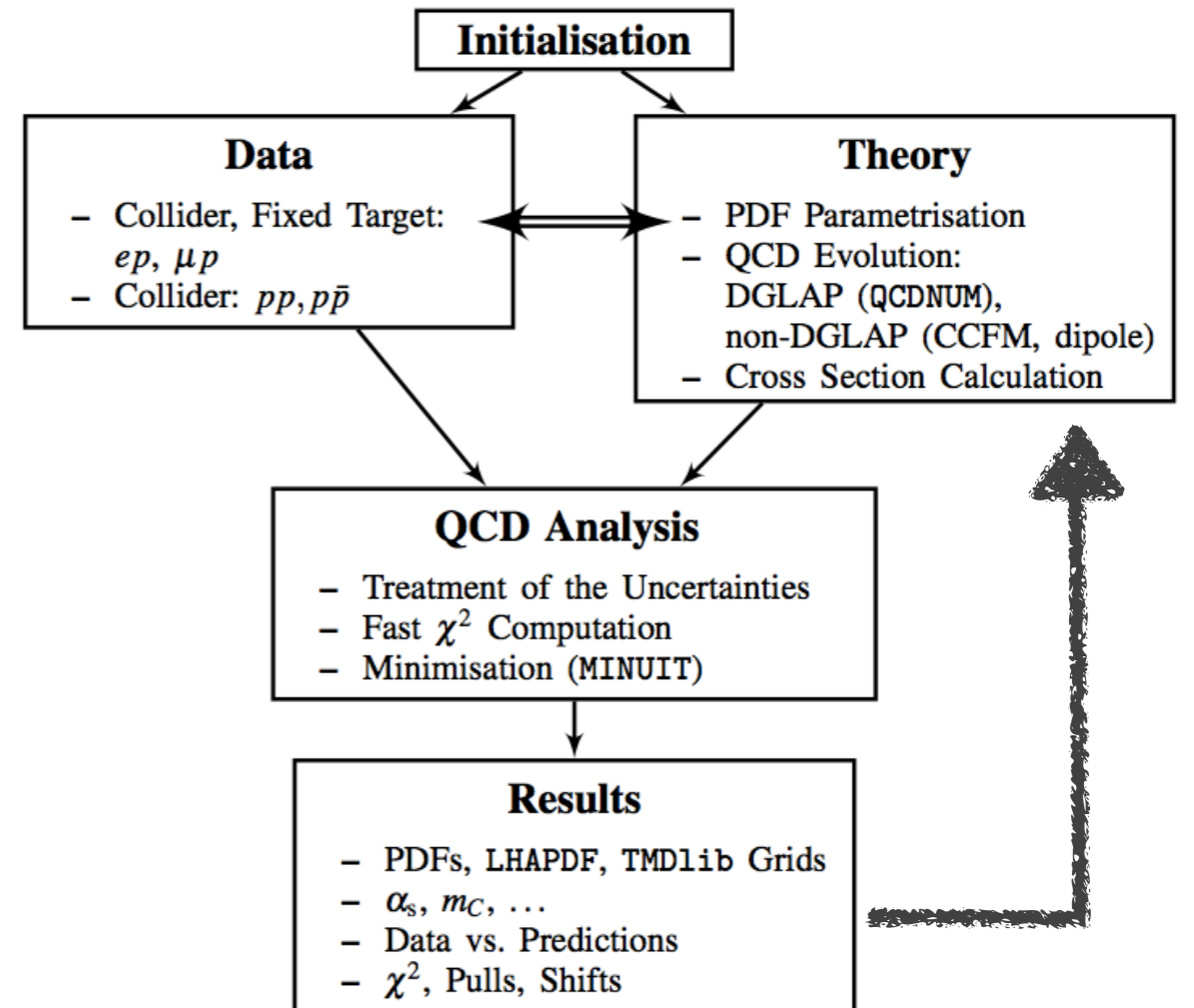
$$\sigma(pp \rightarrow q\bar{q} + X) = \int \frac{dx_{g1}}{x_{g1}} \frac{dx_{g2}}{x_{g2}} \int d^2 k_{t1} d^2 k_{t2} \hat{\sigma}(\hat{s}, k_t, \bar{q}) \times x_{g1} \mathcal{A}(x_{g1}, k_{t1}, \bar{q}) x_{g2} \mathcal{A}(x_{g2}, k_{t2}, \bar{q})$$

# Mechanism of extracting PDFs:

Extraction of PDFs relies on precision measurements to challenge theory

interplay between data and theory

1. Parametrise PDFs at the starting scale
  - multiple options for functional forms
    - Standard Polynomial, Chebyshev, etc
2. Evolve to the scale corresponding to data point
  - QCD(DGLAP) evolution codes [QCDNUM, APFEL]
  - kt ordered evolution, Dipole models, QCD(DGLAP)+QED
3. Calculate the cross section
  - various heavy flavour schemes:
    - RT, ACOT, FONLL, FFNS(ABM)
  - fast grid techniques interfaced to DY:
    - APPLGRID, FASTNLO, APFELgrids
4. Compare with data via  $\chi^2$ :
  - multiple forms to account for correlations
5. Minimize  $\chi^2$  with respect to PDF parameters
  - Profiling, reweighting
  - Fit: MINUIT, data driven regularisation



xFitter EPJC (2015), 75:304

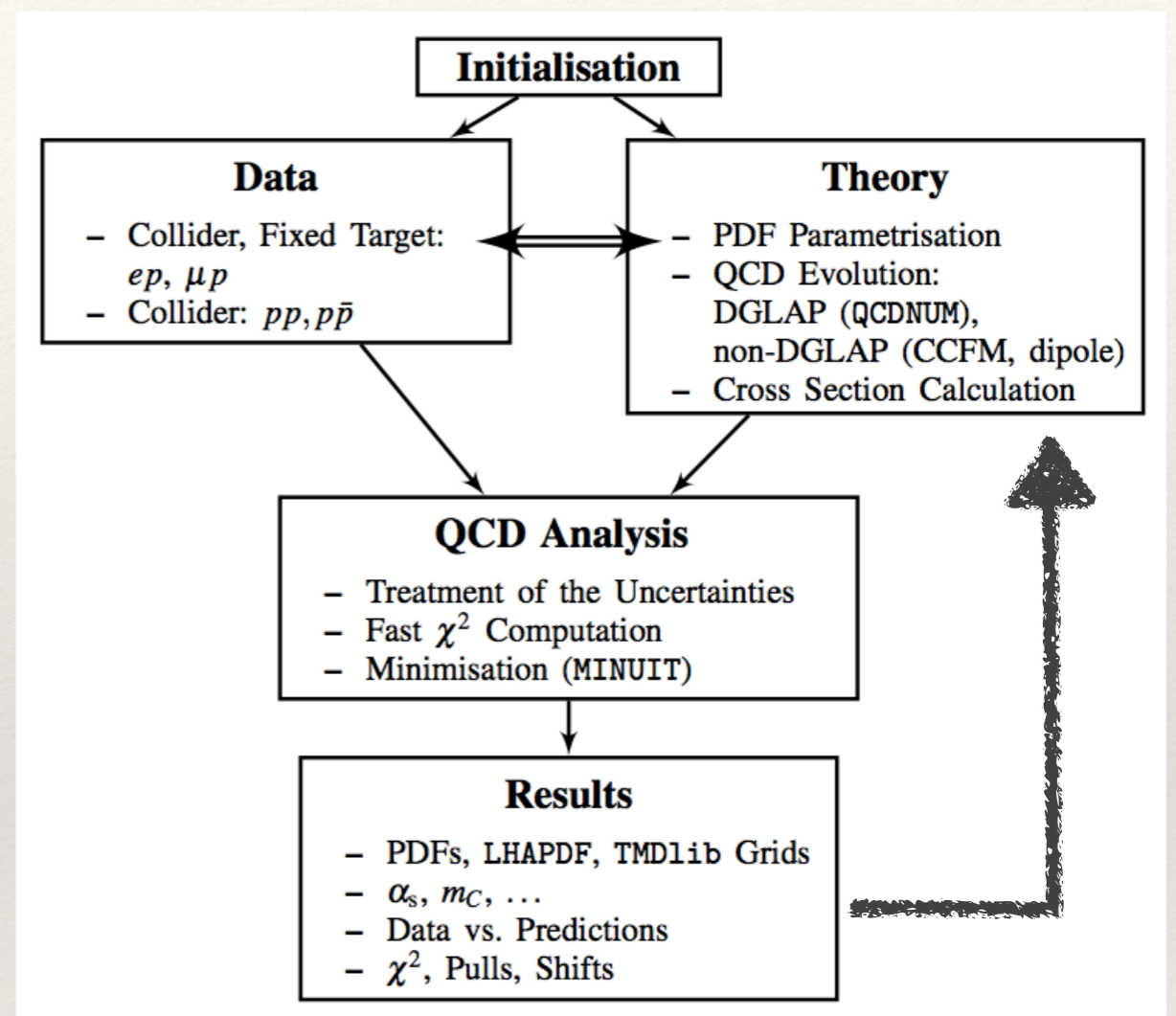
~2000 iterations

[See Ringaile's slides for more details about xFitter]

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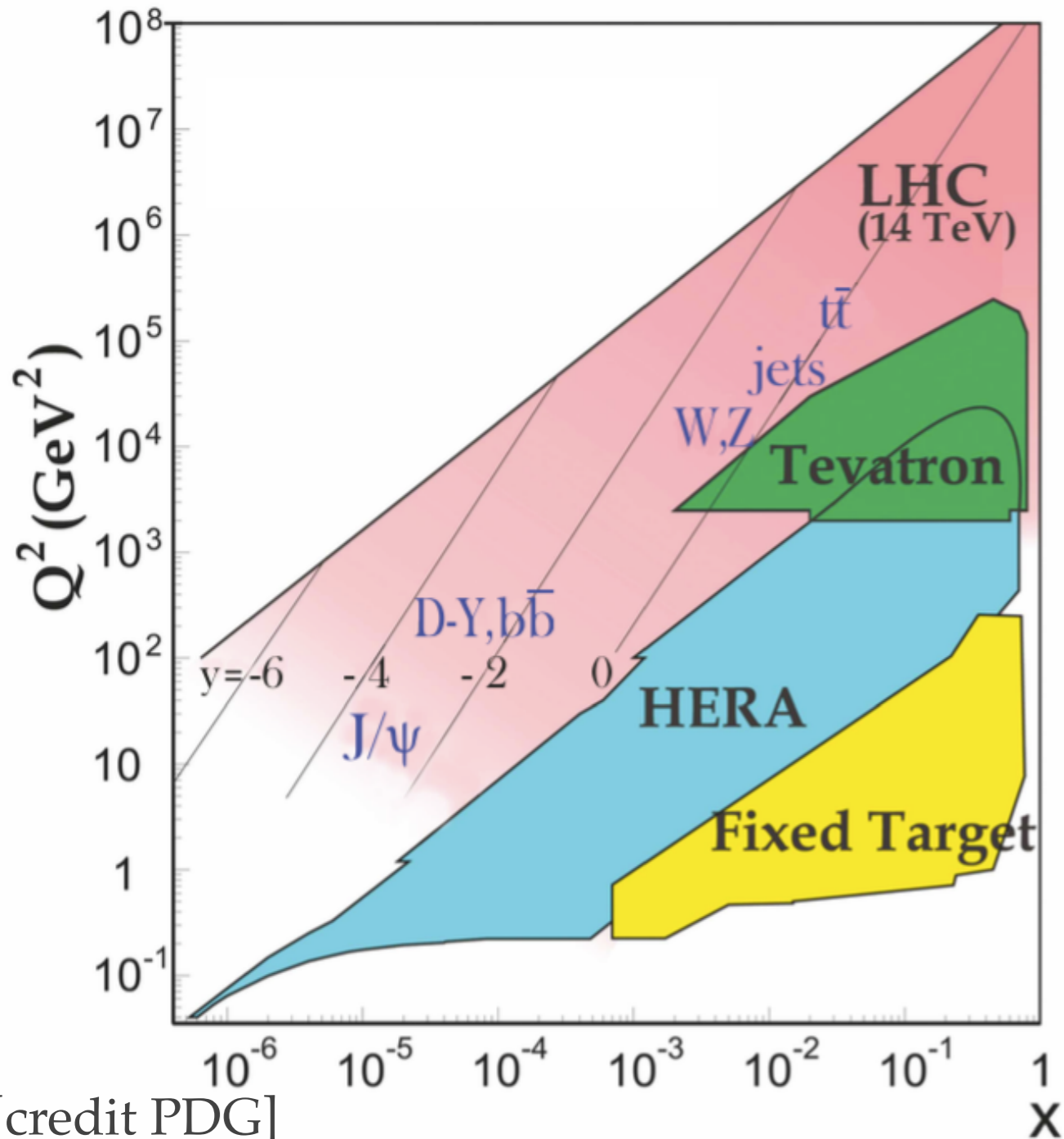
xFitter EPJC (2015), 75:304

~2000  
iterations

[See Valerio's slides for details on APFEL, MELA...]

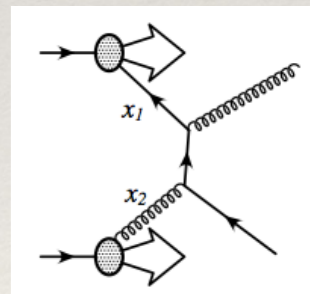
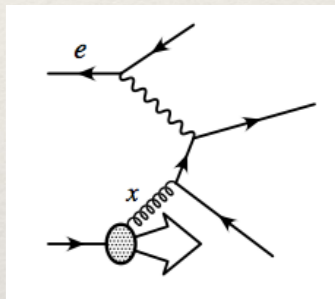
Tools for QCD Fits: xFitter, APFEL, Alpos, OPENQCDRAD, QCDNUM ...

# Data for studying Proton Structure



Persistent experimental effort over the last 40 years both by fixed-target and collider experiments around the world supported by the intense theoretical developments

- The cleanest way to probe Proton Structure is via Deep Inelastic Scattering [DIS]:
- Precision of proton structure can be complemented by the Drell Yan [DY] processes at the collider experiments



$Q^2$ : resolving power of experiment  
 $x$ : fraction of proton's momentum

Multiple precision measurements from Fixed target, HERA, Tevatron, and LHC

Many groups to analyse these data and interpret them

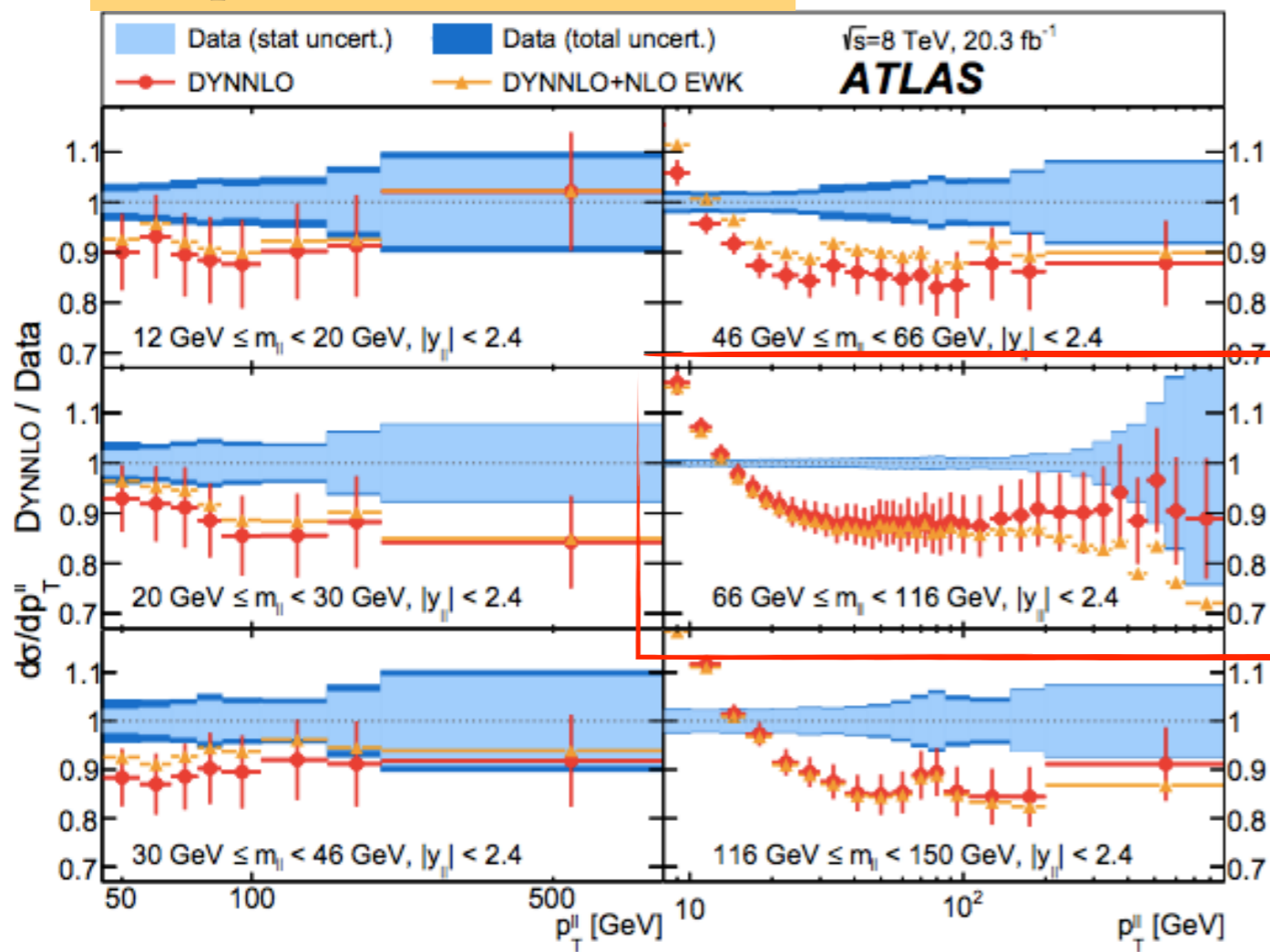
# Vector boson pT spectrum at the LHC

ATLAS and CMS both measured and studied the Z pT spectrum in rapidity bins:

**high pT region:** fixed order calculations up to  $O(\alpha_s^2)$  and now even  $O(\alpha_s^3)$  + EW corrections

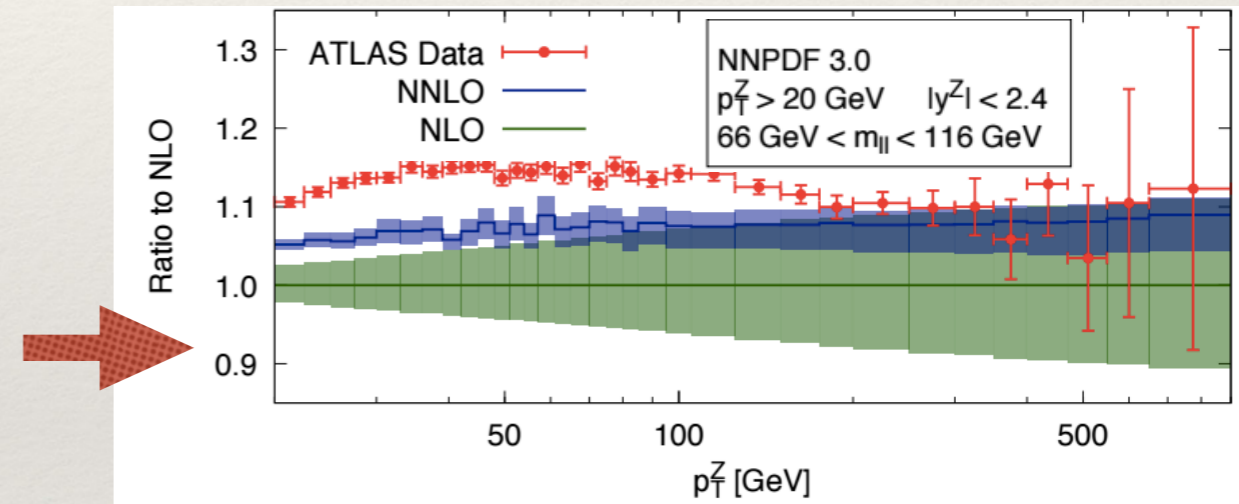
comparison to fixed order:

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Higher Order corrections would improve data - theory agreement

*arxiv:1605.04295*



Measurement with constraining powers for PDFs and alphas

# Vector boson $p_T$ spectrum at the LHC

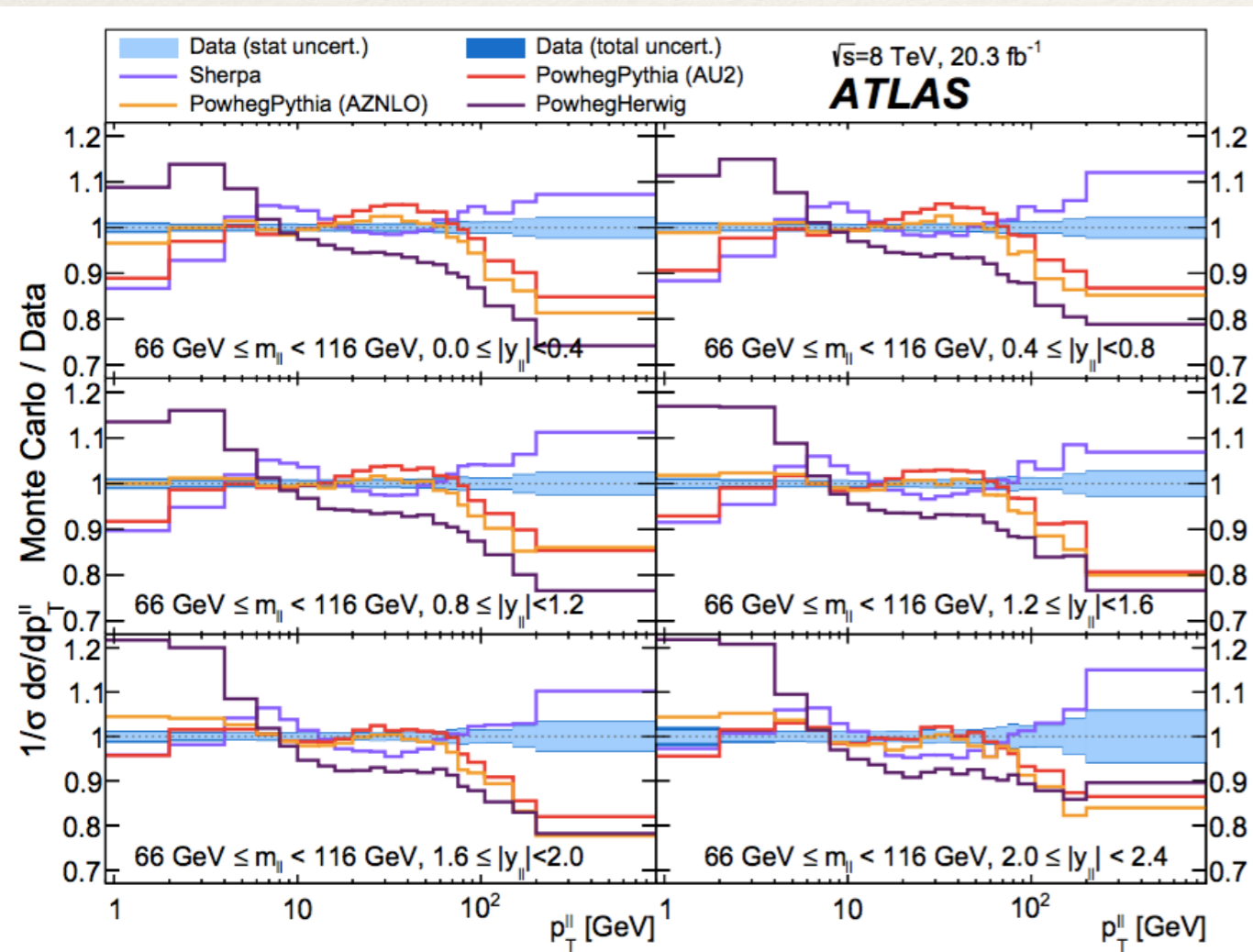
ATLAS and CMS both measured and studied the Z  $p_T$  spectrum in rapidity bins

**low  $p_T$  region:** dominated by the emission of soft gluons

—> fixed order calculations don't work —> need resummation and shower models

comparison to MC:

Precise data for MC tuning!



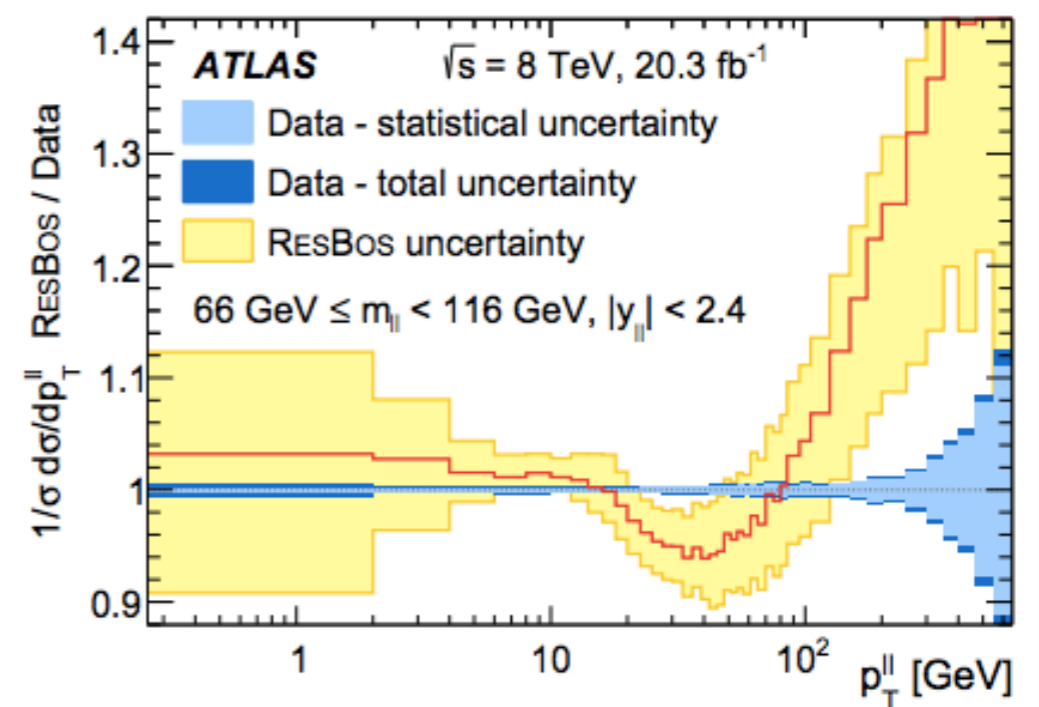
$66 \text{ GeV} \leq m_{\parallel} < 116 \text{ GeV}$

MC with different PS models are compared

❖ Powheg+Pythia AZNLO [tuned to 7 TeV Z  $p_T$ ]

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comparison to resummed calculations:





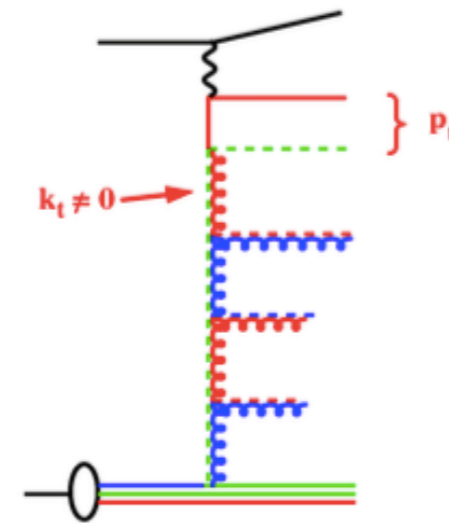
# Transverse Momentum Distributions

- ❖ Fixed order calculations don't always work and in order to improve the quality of PDF fits in small/high  $x$  regions
  - > a challenge to merge DGLAP, BFKL, cascade evolutions
- ❖ TMDs were first introduced at small  $x$  as unintegrated gluon PDFs
  - ❖ intrinsic at small  $k_T$
  - ❖ perturbative evolution at large  $k_T$
- ❖ However, the concept is now extended to the full kinematic space and to all quark species

[see Hannes slides]

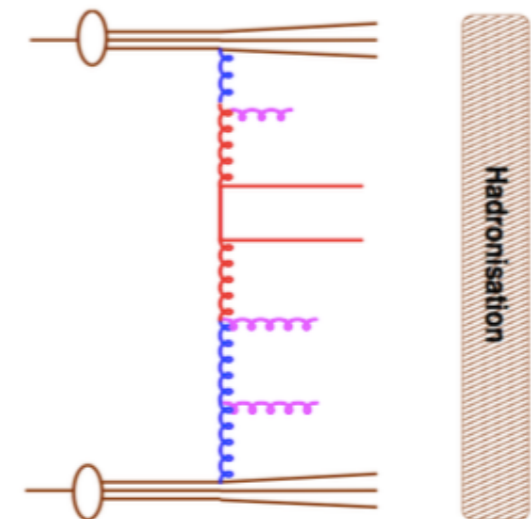
- in ep scattering:

$$\sigma(ep \rightarrow e'X) = \int dx_g/x_g [d^2 k_t x_g \mathcal{A}_i(x_g, k_t, \bar{q})] \times \hat{\sigma}(x_g, k_t, x, \bar{q}, Q^2)$$



- in pp scattering

$$\sigma(pp \rightarrow q\bar{q} + X) = \int \frac{dx_{g1}}{x_{g1}} \frac{dx_{g2}}{x_{g2}} \int d^2 k_{t1} d^2 k_{t2} \hat{\sigma}(\hat{s}, k_t, \bar{q}) \times x_{g1} \mathcal{A}(x_{g1}, k_{t1}, \bar{q}) x_{g2} \mathcal{A}(x_{g2}, k_{t2}, \bar{q})$$



# Transverse Momentum Distributions

MC simulation combines fixed order partonic calculations with PS and hadronisation

—> needs reshuffling of kinematic variables after PS generations

—> **TMDs are introduced for a proper simulation of parton showers:**

- generalisation of QCD factorisation with an explicit dependence on transverse momentum and polarisations

$$\sigma(pp \rightarrow q\bar{q} + X) = \int \frac{dx_{g1}}{x_{g1}} \frac{dx_{g2}}{x_{g2}} \int d^2 k_{t1} d^2 k_{t2} \hat{\sigma}(\hat{s}, k_t, \bar{q}) \times x_{g1} \mathcal{A}(x_{g1}, k_{t1}, \bar{q}) x_{g2} \mathcal{A}(x_{g2}, k_{t2}, \bar{q})$$

- they obey the evolution equations which generalise the ordinary RGE of collinear PDFs
  - ❖ solved using MC
  - ❖ reformulated using separate kernels gluons from sea quarks
    - ❖ —> perform the evolution separately

# Transverse Momentum Distributions evolved using MC method

## MC code

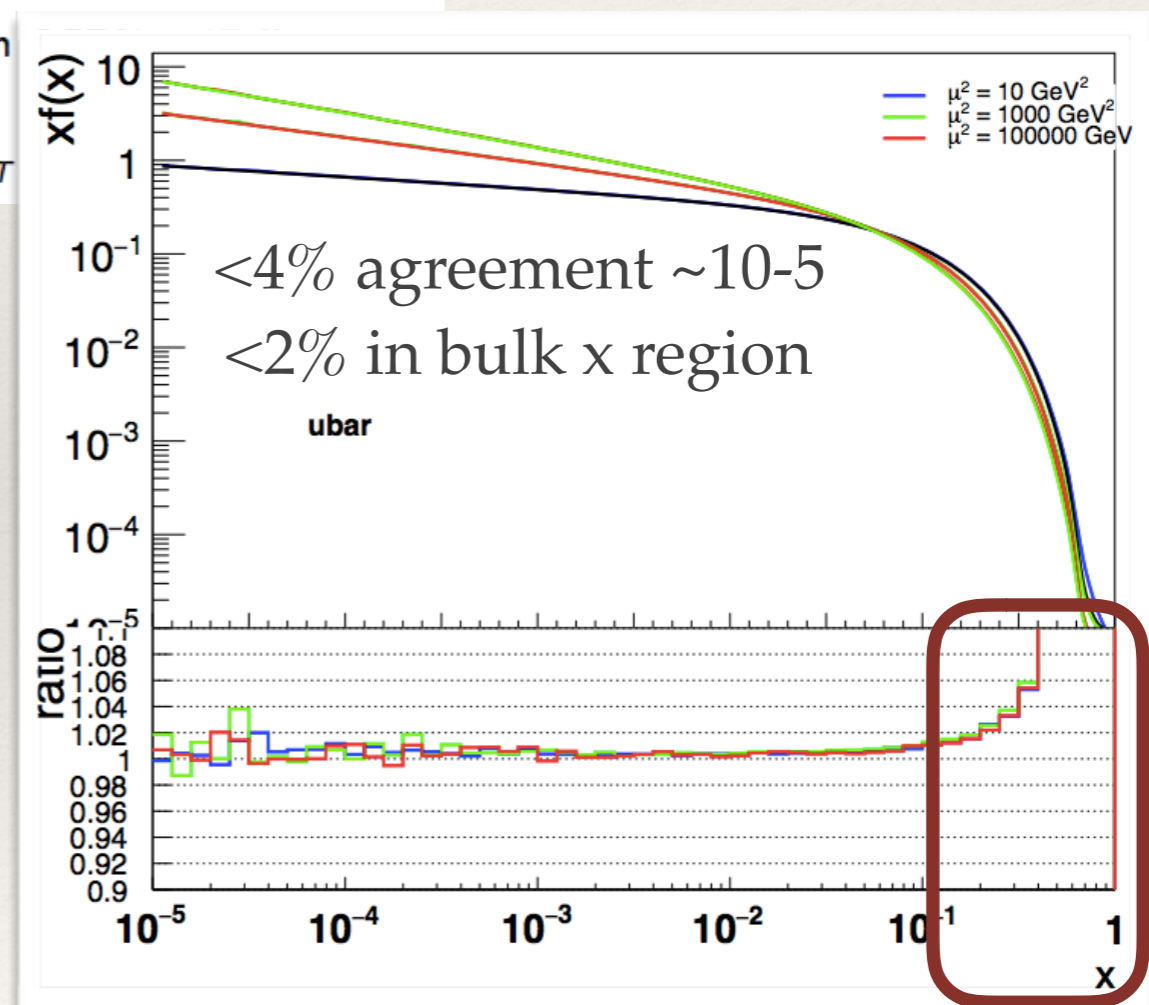
In this presentation: MC results obtained with updated and improved [uPDFevolv code](#):

- ▶ full coupled quark and gluon DGLAP evolution (gluon, sea and valence evolution),
- ▶ fixed flavour number scheme,
- ▶ LO in  $P(z)$ ,
- ▶ 1-loop- $\alpha_s$  (but also 2-loop- $\alpha_s$  implemented),
- ▶  $xf(x, t)$ ,
- ▶ the initial distributions for  $u, d, s, \dots, \bar{u}, \bar{d}, \bar{s}, \dots$  and gluon come from other parametrization can be used).

Evolution over the whole range in  $x$ ,  $Q^2$  and all kinematically allowed  $k_T$

A sample of validation plots:  
Analytical integration vs MC of  
solving DGLAP

[see Ola's slides for more]



due to  
grid

# TMDs in xFitter: implementation

Steering block:

assign which evolution to be used  
assign initial values for fitted parameters

Initialise theory

Evolve initial objects

Calculate Observables (SFs, Xsec)

minimize the chi2

QCDNUM

block for  
storing output of PDFs for display

Currently in xFitter:

```
'DGLAP' ! 'DGLAP' -- collinear evolution
! 'DGLAP_APFEL' -- collinear evolution with APFEL
! 'DGLAP_QEDEVOL' -- collinear evolution with QEDEVOL
! 'DGLAP_APFEL_QED' -- collinear evolution with APFEL with QED corrections
! 'DGLAP_TMDEVOL' -- collinear TMD evolution
! 'DIPOLE' -- dipole model
! 'uPDF' -- un-integrated PDFs
!uPDF1 fit with kernel ccfm-grid.dat file
!uPDF2 fit evolved uPDF, fit just normalisation
!uPDF3 fit using precalculated grid of sigma hat
```

```
external LHAPDFsubr
external APFELsubr
external APFELsubrPhoton
external QEDEVOLsubr
external TMDEVOLsubr
```

# Toolkit: TMDs in xFitter implementation

## Steps in implementations:

- A. create a new module which can be steerable via configure flag
  - `./configure -- enable-NEWMODULE`
- B. Add new option in the steering card
  - `TheoryType = 'DGLAP_TMDEVOL' ! 'DGLAP' -- colinear TMD evolution`
- C. Interfacing the new module to xFitter:
  1. reading the steering card
    - `src/read_steer.f`: it requires new internal index
  2. initialise evolution:
    - `src/init_theory.f`: call `NEWMODULE_ini` assigned to the new index
  3. create a routine that sets all input parameters of your new routine (passing of the inputs) and protect against the case when the module is not linked (can be done via configure commands)
  4. during the evolution: skip the default evolution which is taken from QCDNUM
    - assign the `IPDFSET > 6` (external PDFs to QCDNUM)
  6. PDF decomposition -> transform them into basis of your choice to be passed into your code
    - create a new subroutine stored in `src/evolution.f`
  7. Storing/Filling the grids:
    - done on `src/evolution.f` via call from QCDNUM
    - call `PDFEXT(NEWMODULE_subr,IPDFSET,dble(0.001),epsi)`

Steering block:  
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QCDNUM  
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# QCD Settings for iTMD extraction

The QCD settings are optimised for HERA measurements of proton structure functions:

PDFs are parametrised at the starting scale  $Q_0^2=1.9 \text{ GeV}^2$  as follows: [arXiv:1506.06042](https://arxiv.org/abs/1506.06042)

$$\begin{aligned}
 xg(x) &= A_g x^{B_g} (1-x)^{C_g} - A'_g x^{B'_g} (1-x)^{C'_g}, \\
 xu_v(x) &= A_{uv} x^{B_{uv}} (1-x)^{C_{uv}} (1 + E_{uv} x^2), \\
 xd_v(x) &= A_{d_v} x^{B_{d_v}} (1-x)^{C_{d_v}}, \\
 x\bar{U}(x) &= A_{\bar{U}} x^{B_{\bar{U}}} (1-x)^{C_{\bar{U}}} (1 + D_{\bar{U}} x), \\
 x\bar{D}(x) &= A_{\bar{D}} x^{B_{\bar{D}}} (1-x)^{C_{\bar{D}}}.
 \end{aligned}$$

  fixed or constrained by sum-rules  
  parameters set equal but free

**NC structure functions**

$$F_2 = \frac{4}{9} (xU + x\bar{U}) + \frac{1}{9} (xD + x\bar{D})$$

$$xF_3 \sim xu_v + xd_v$$

**CC structure functions**

$$W_2^- = x(U + \bar{D}), \quad W_2^+ = x(\bar{U} + D)$$

$$xW_3^- = x(U - \bar{D}), \quad xW_3^+ = x(D - \bar{U})$$

—> 14 free parameters after imposing Sum Rules, and assumption that  $x_{\text{ubar}}=x_{\text{dbar}}$   $x \rightarrow 0$

- ❖ TMDs are evolved via MC evolution equations to LO ( $\alpha_s(M_Z)=0.118$ )
- ❖ Thorne-Roberts GM-VFNS for heavy quark coefficient functions – as used in MMHT
- ❖  $\chi^2$  definition used in the minimisation [MINUIT] accounts for correlated uncertainties:

$$\chi_{\text{exp}}^2(m, s) = \sum_i \frac{[m^i - \sum_j \gamma_j^i m^i s_j - \mu^i]^2}{\delta_{i,\text{stat}}^2 \mu^i m^i + \delta_{i,\text{uncor}}^2 (m^i)^2} + \sum_j s_j^2$$

m - th prediction  
 $\mu$  - data  
 s - sys shift

# Propagation of experimental uncertainties to iTMDs

There are two standardised approaches to propagate the exp. uncertainties:

- ❖ Hessian Eigenvectors: based on expansion of the  $\chi^2$  function

$$\Delta\chi^2 = \chi^2 - \chi_0^2 = \sum_{i=1}^d \sum_{j=1}^d H_{ij} (a_i - a_i^0) (a_j - a_j^0)$$

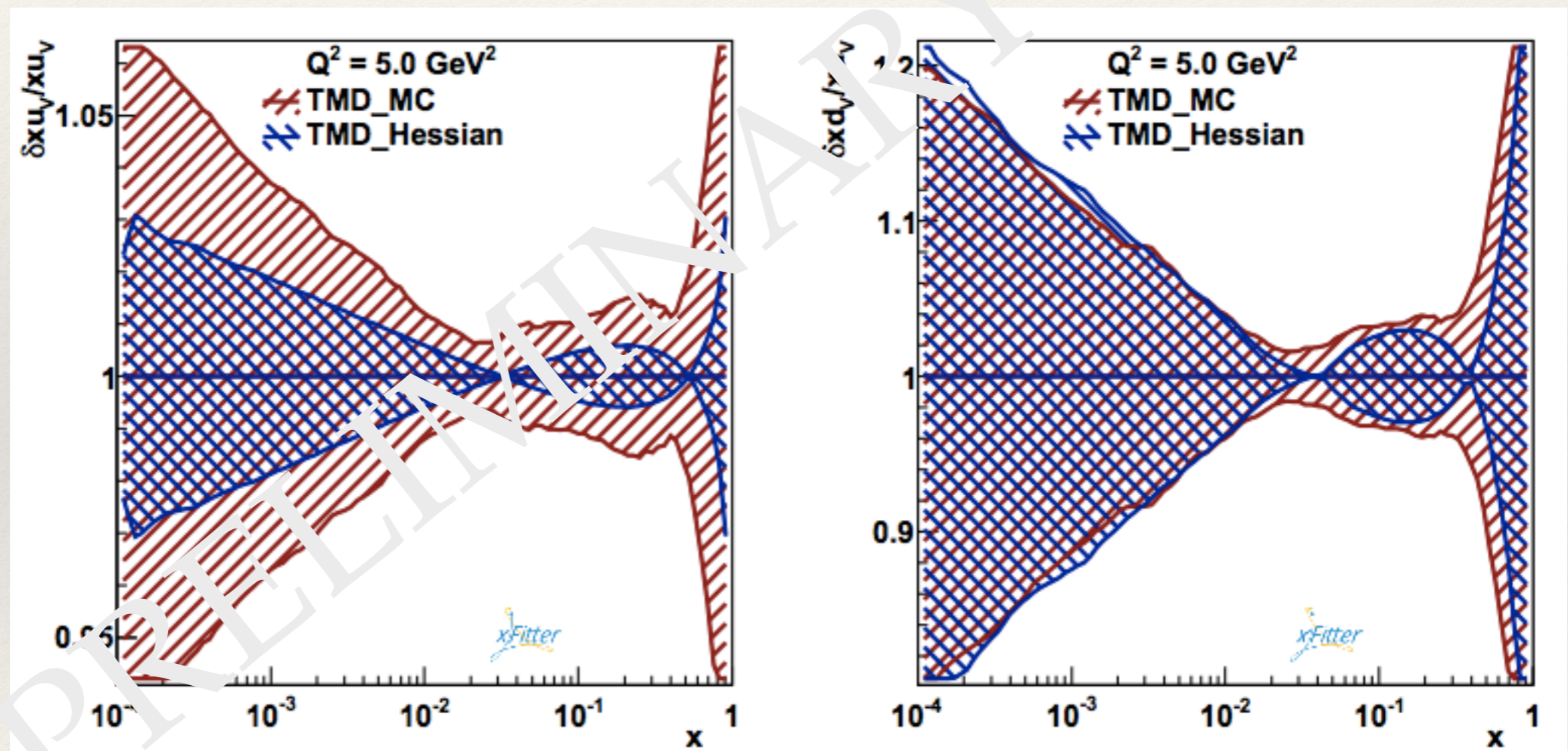
PDF parameters:  $\{a_i\}_{i=1\dots d}$

Hessian matrix of second derivatives:  $H_{ij} = \frac{1}{2} \frac{\partial^2 \chi_{\text{global}}^2}{\partial a_i \partial a_j} \Big|_0$

- ❖ in xFitter:  $\Delta\chi^2 = 1$  for one sigma (68% CL)
- ❖ Monte Carlo Replica:
  - ❖ generation of replicas of experimental data by smearing the central values of data points by statistical and systematical uncertainty (accounting for the correlations)
  - ❖ perform a separate fit using each data replica

# First LHAPDF TMD for full kinematic plane

it can be distributed using **Hessian Error** estimation or **Monte Carlo Replica**



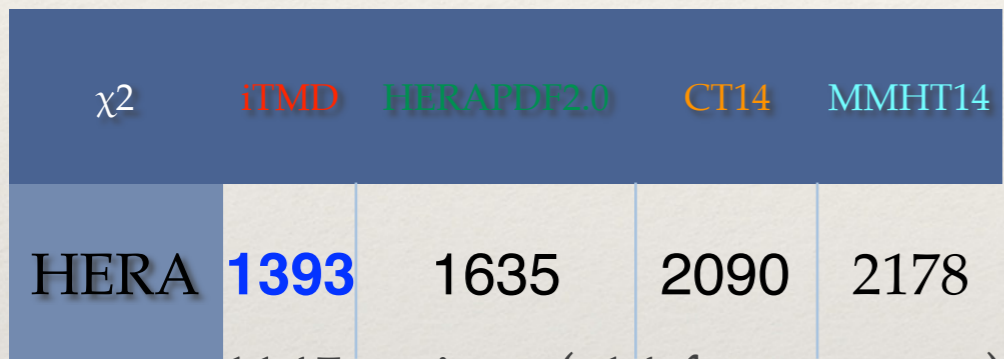
MC error estimation is generally more robust

→ LHgrid that can be plugged in any other application

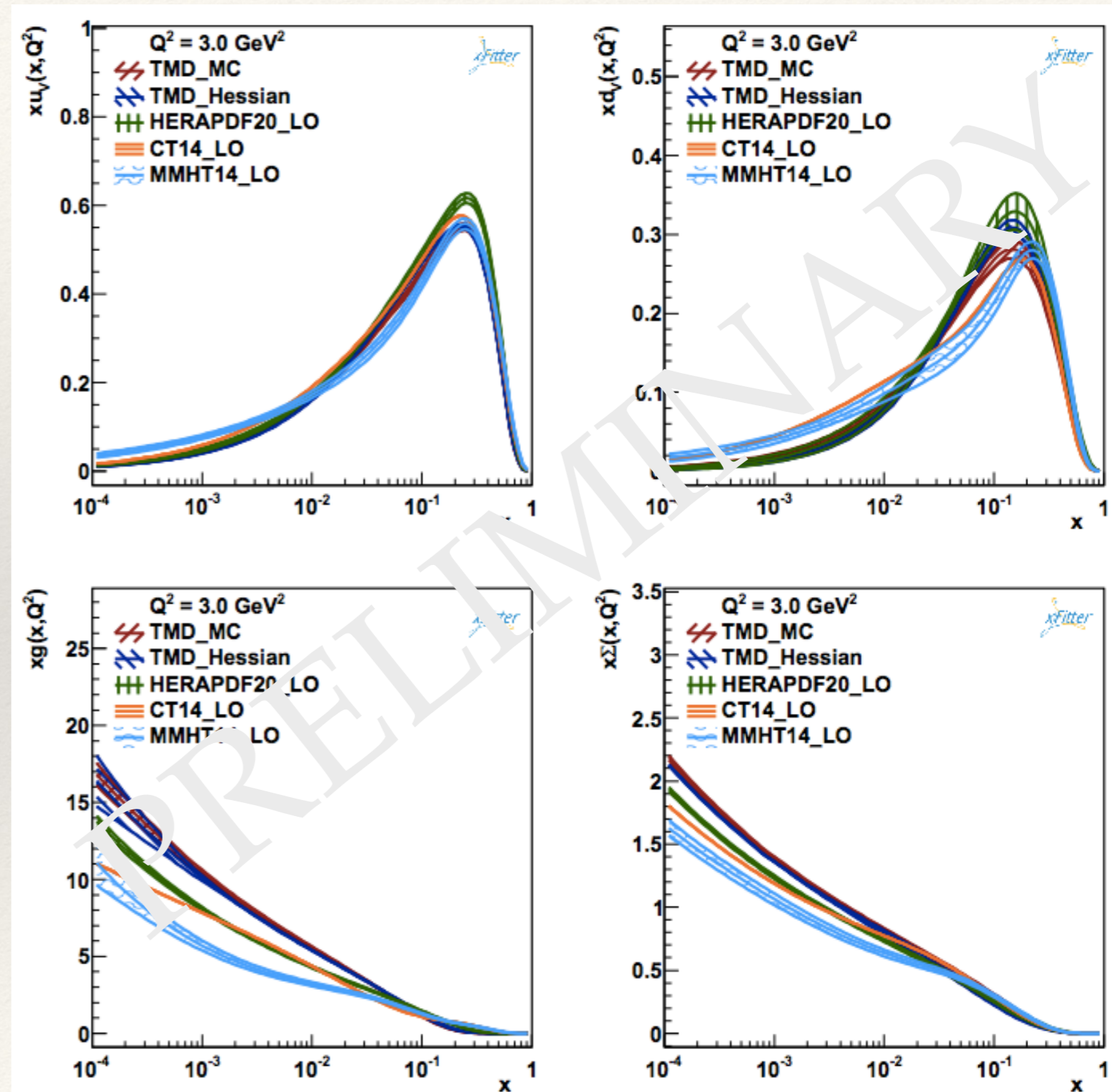


# First LHAPDF TMD for full kinematic plane

Integrated PDFs from TMD evolution using MC method  
(compared with standard LO PDFs)



[not including PDF uncertainties]

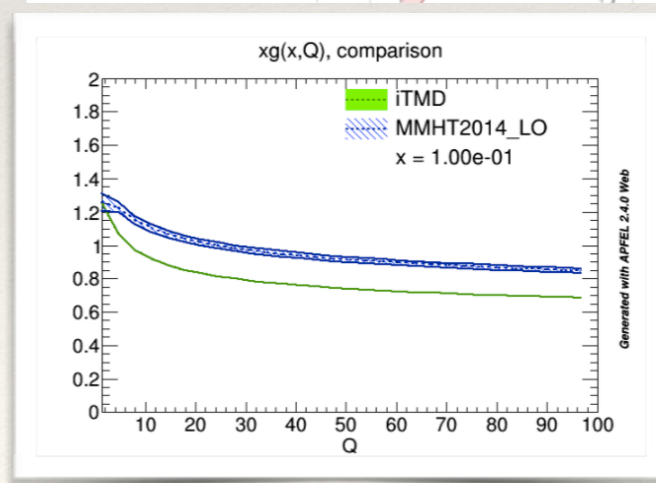


—> LHgrid that can be plugged in any other application

# Example: using tmdplotter or apfel web interface

❖ TMDplotter <http://tmdplotter.desy.de>

❖ APFEL <http://apfel.mi.infn.it/>



[see Valerio's slides]

# Summary

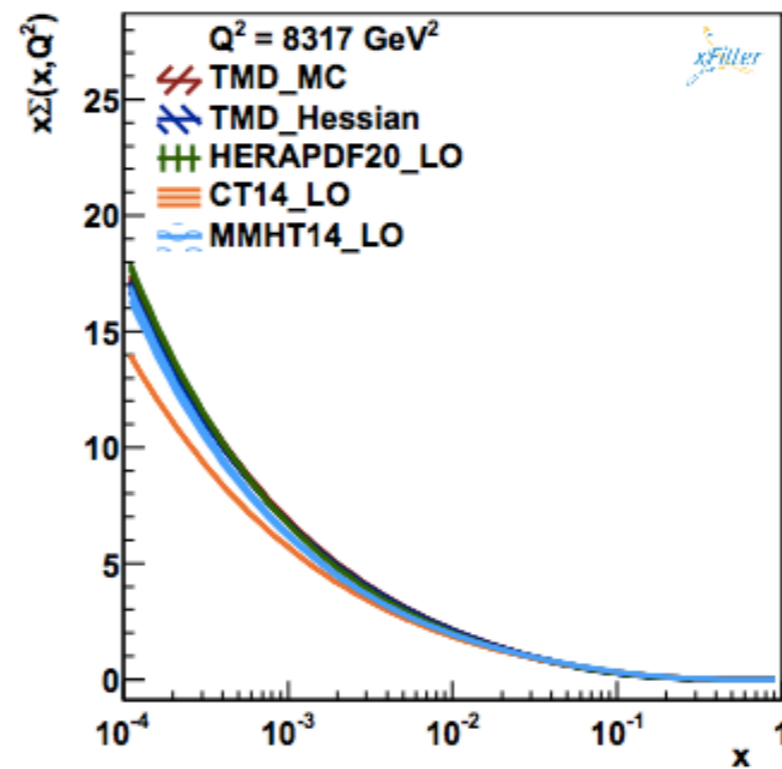
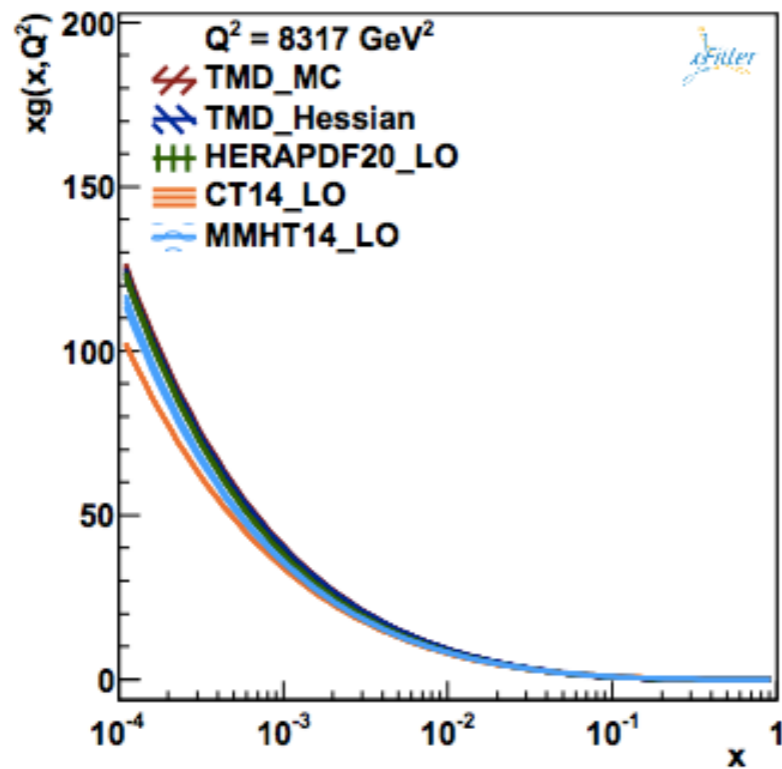
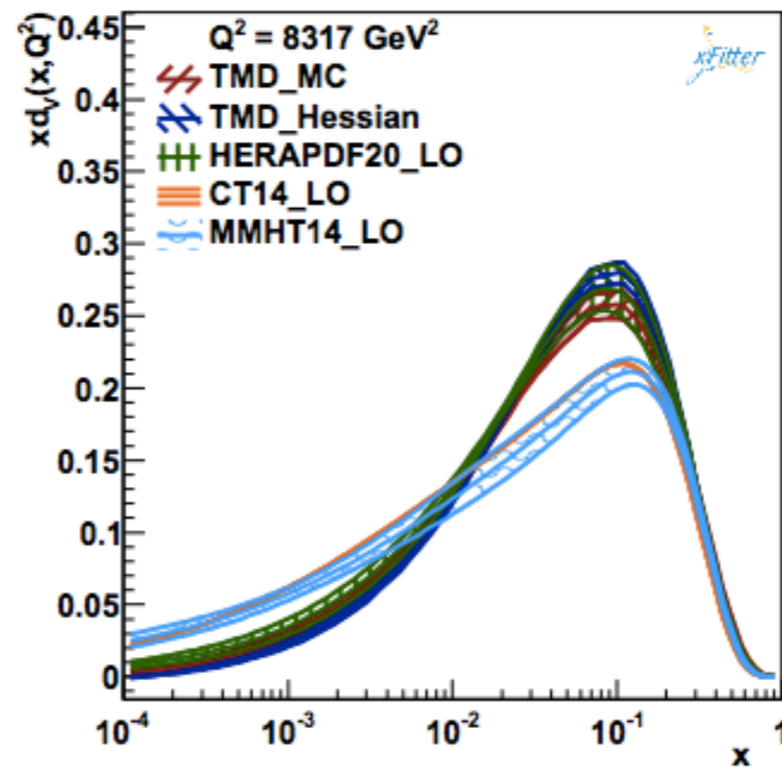
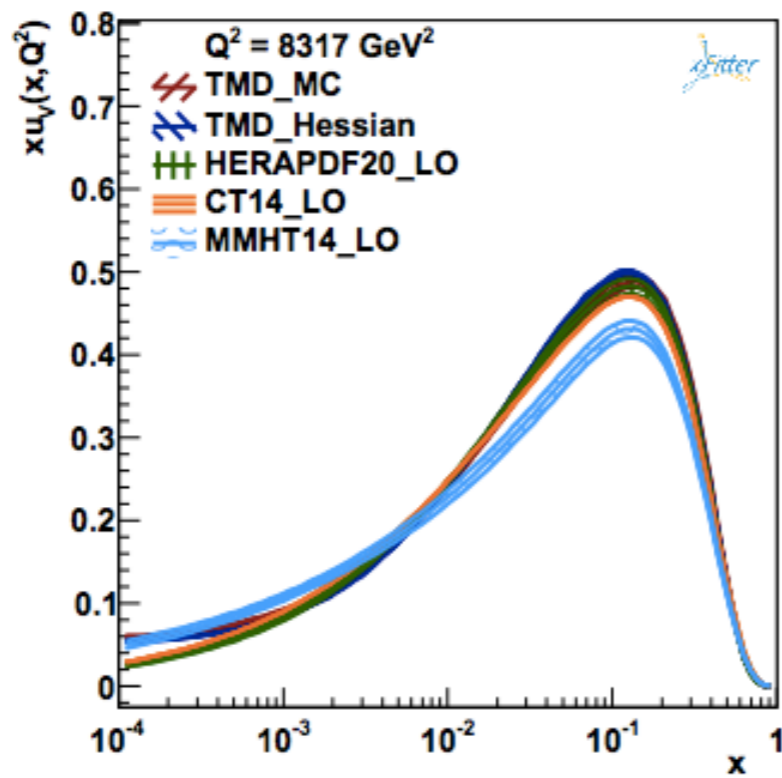
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- ◆ The precision measurements at the LHC dictate for more scrutiny to allow for an interpretation in the context of QCD:
  - ◆ many observables suffer from a lack of a complete data modelling in a concise matter in a full kinematic phase space
- ◆ TMDs can be expanded from their role in the low  $x$  region to the full kinematic space for all quark species:
  - ◆ a first TMD using MC solution for DGLAP evolution at LO with experimental uncertainties estimated using replica or hessian methods has been extracted using xFitter QCD platform - a promising new avenue to provide a consistent modeling of the experimental data (from low to high  $p_t$ )
    - ◆ fits based on DIS data from HERA
  - ◆ the iTMDs are automatically produced in LHAPDF grid formats
  - ◆ next goal is to extend the solution to NLO

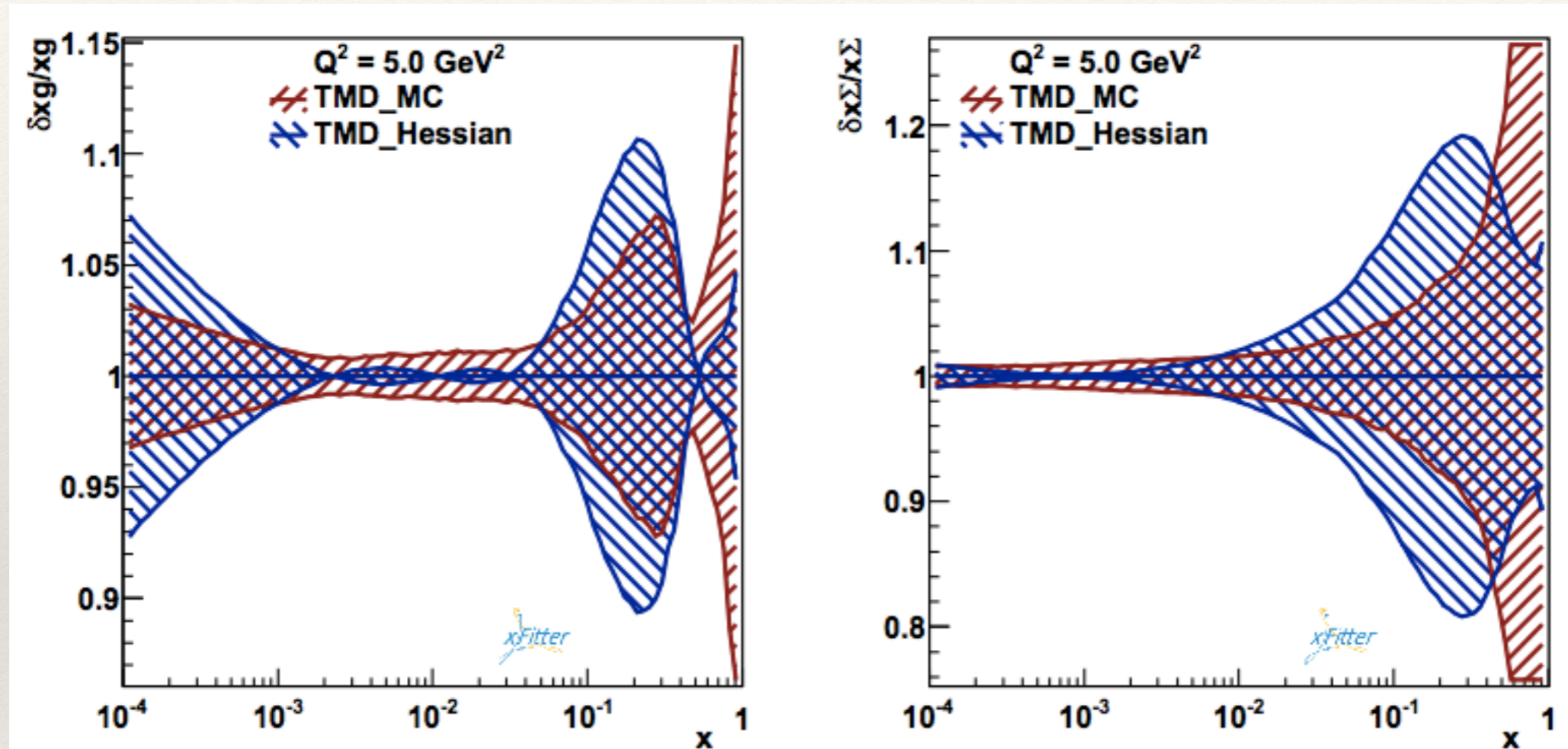
Thank you!



# integrated TMDs vs global PDFs



# MC vs Hessian uncertainties

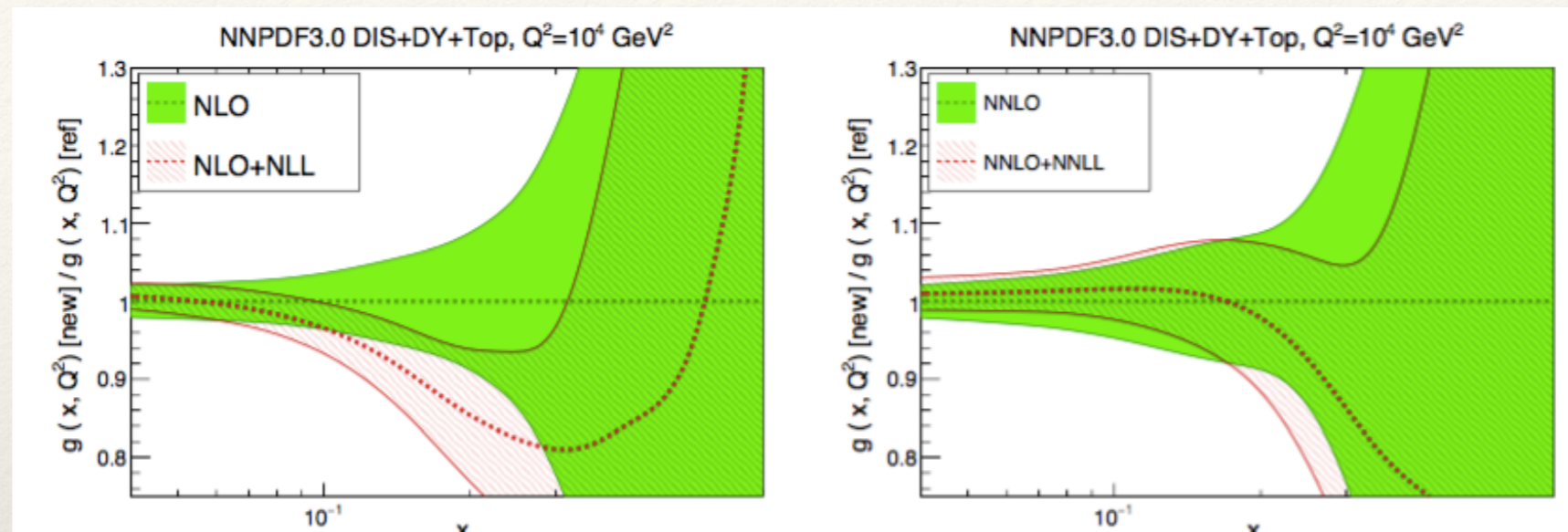


# New developments: PDFs from resummed calculations

- Fixed order calculations don't always work and in order to improve the quality of PDF fits in small/high  $x$  regions there have been efforts in providing PDFs consistent with Resummed Computations

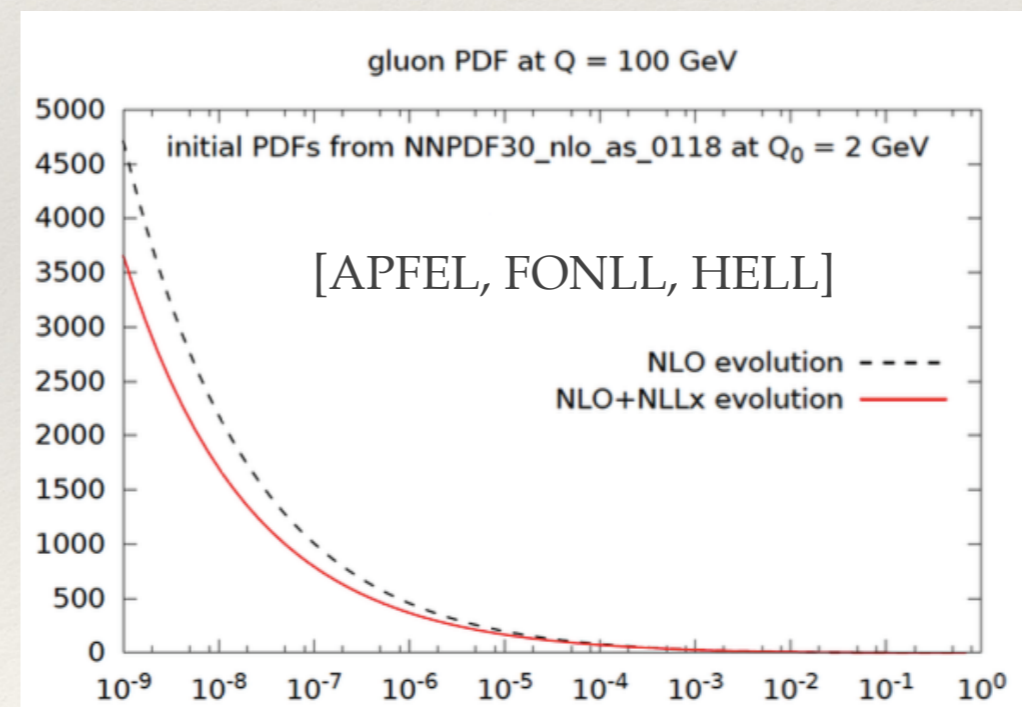
[using NNPDF framework]

- PDF fits with threshold resummation tested [high  $x$ ]
  - sizeable effect at NLO+NLL, smaller effect at NNLO+NNLL



- PDF fits with high-energy resummation show promising results [low  $x$ ]
  - NLO+NLL $x$  evolution

[ref: M. Bonvini QCD@LHC2016]

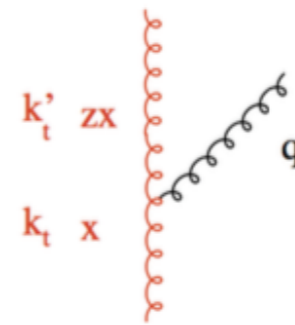


It would be interesting to see the effects combined: PDFs with resummed threshold and high-energy

- Evolution consists of step-by-step simulation of individual branchings
  - at each branching, exact energy-momentum conservation is applied, including  $k_t$

$$\vec{k}'_t = \vec{k}_t + \vec{q}_t$$

- with this, a TMD can be constructed, once  $q_t$  is known
- evolution happens in  $q_t$  (for DGLAP) case with  $q'_t \gtrsim q_t$ 
  - evolution in CCFM would be different ..
- since only real splittings are simulated,  $z_{max}$  must be specified for splitting function.



- virtual corrections are correctly treated with Sudakov form factor (see presentation by Ola at Dubna meeting)
- Apart from TMD densities, automatically (integrated) collinear densities are obtained:
  - evolution itself does not depend on  $k_t$
- $k_t$  enters the kinematics from the x-section only

## new version:

- ▶ full coupled quark and gluon DGLAP evolution (gluon, sea and valence evolution)
- ▶ fixed flavour number scheme (only u,d,s)
- ▶ LO in  $P(z)$  (we plan to have NLO in  $P(z)$ ),
- ▶ 1-loop- $\alpha_s$  (but also 2-loop- $\alpha_s$  implemented).
- ▶  $xf(x, t)$  ,

Evolution over the whole range in  $x$ ,  $Q^2$  and all kinematically allowed  $k_T$ .

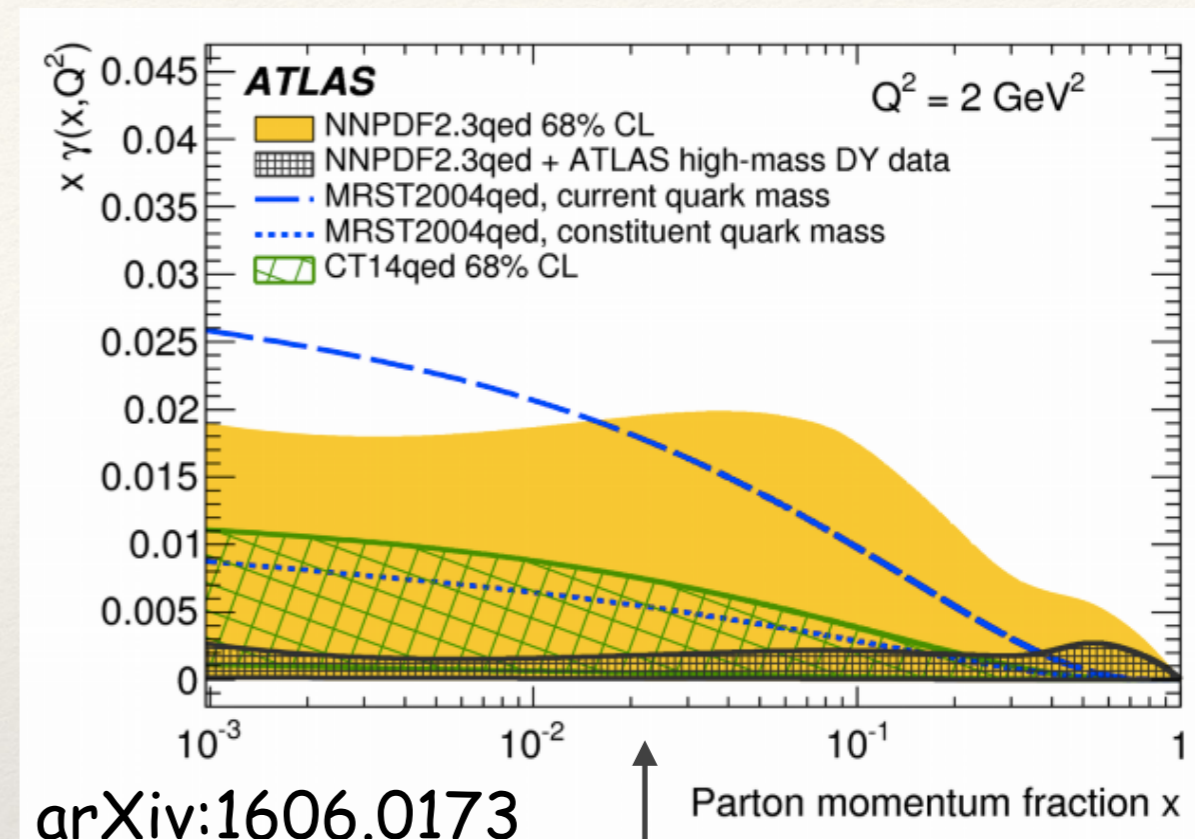


# New Developments for PDF extraction: photon PDF

❖ It starts to become relevant implementation of combined QCD+QED evolution in determining a complete set of PDFs including photon PDFs.

❖ **Studies that account for the photon PDF:**

- ❖ Gluck, Pisano, Reya 2002
- ❖ MRST2004 QED
- ❖ NNPDF2.3 QED → NNPDF3.0 QED
  - ❖ fit to data
- ❖ CT14 QED, CT14 QED\_inc
- ❖ Harland-Lang, Khoze, Ryskin 2016
- ❖ LUXqed 2016: Manohar, Nason, Salam, Zanderighi
  - ❖ use ep scattering and construct a hypothetical model for neutral lepton



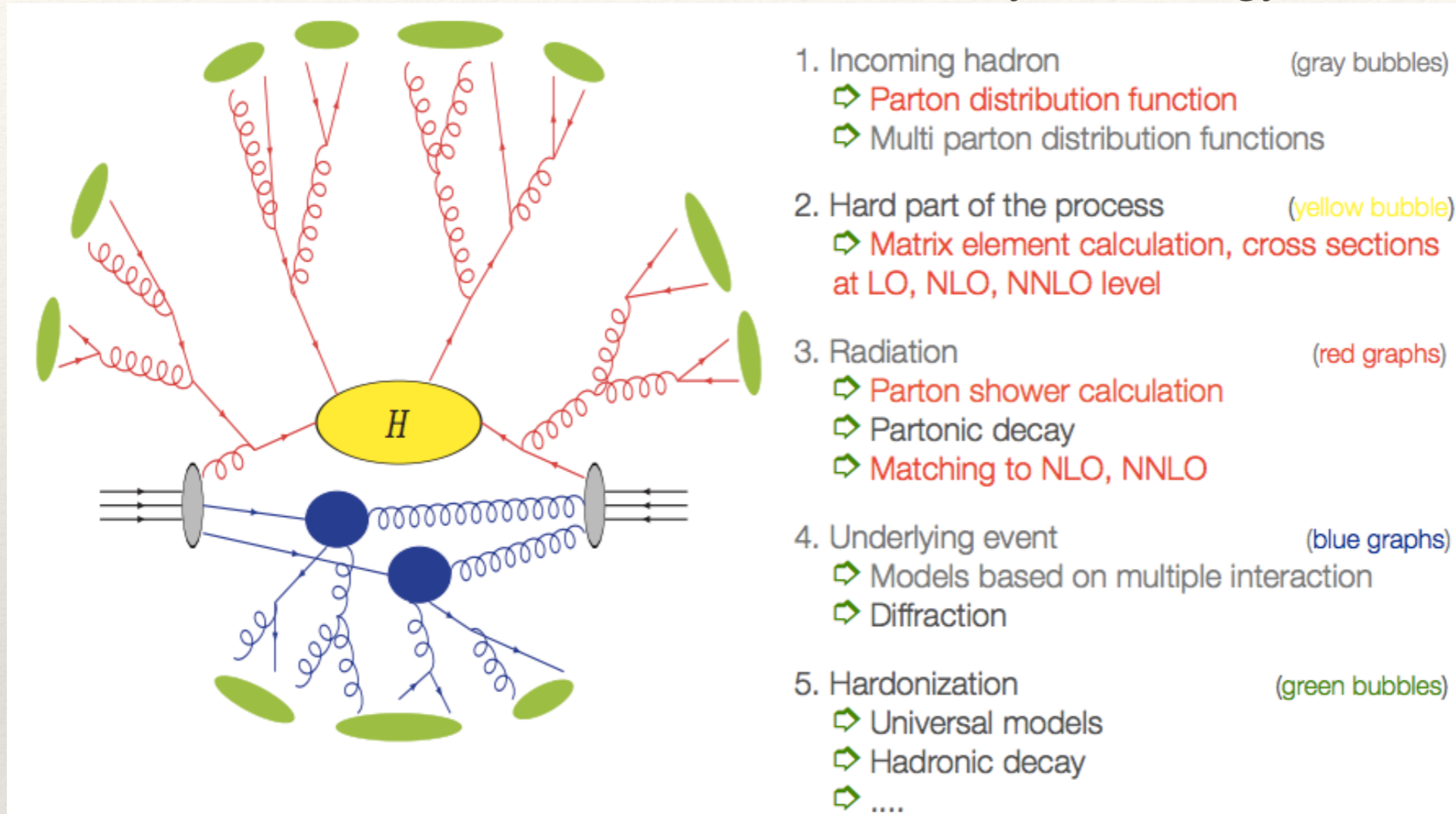
arXiv:1606.0173

Data has a lot of potential



# Roles of PDFs in MC tuning

## ❖ Structure of an event at the LHC (courtesy of Z. Nagy)



### Perturbative framework:

- ❖ LO: easy to calculate: several matrix element generators are available:
  - ❖ ALPGEN, HELAC, MADGRAPH, SHERPA
  - ❖ Strong dependence on the unphysical scales
  - ❖ well defined with LO PDF
- ❖ NLO is the New Standard: HELAC, MADGRAPH, SHERPA+BLACKHAT, AUTODIPOLE, TEVJET, AMC@NLO
  - ❖ The scale dependence can be still big in some processes
- ❖ NNLO & NkLO: Resummation - Parton Showers: POWHEG

# New Developments for PDF extraction: photon PDF

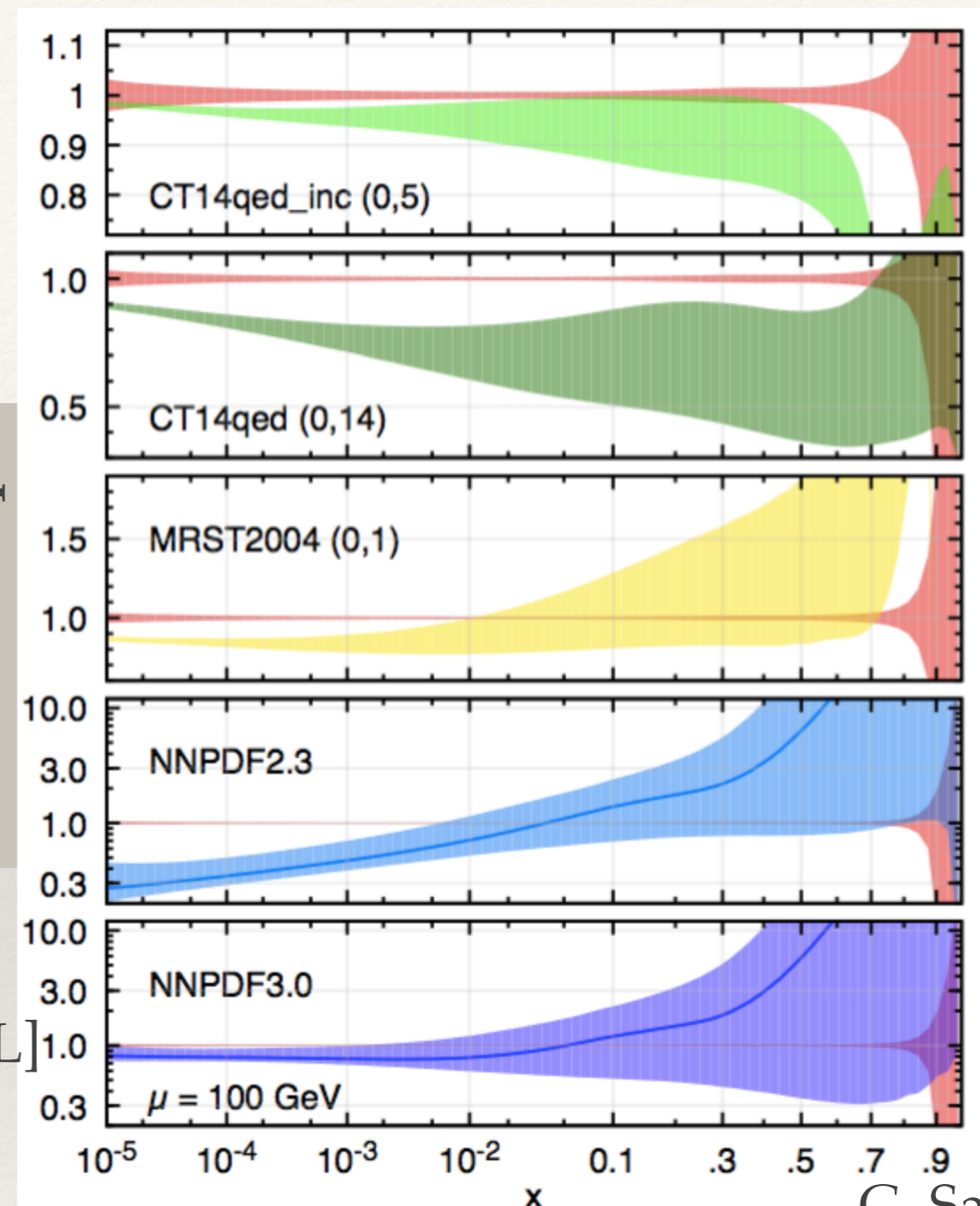
- ❖ It starts to become relevant implementation of combined QCD+QED evolution in determining a complete set of PDFs including photon PDFs.

limited experimental  
constraints

- ❖ **Studies that account for the photon PDF:**

- ❖ Gluck, Pisano, Reya 2002
- ❖ MRST2004 QED
- ❖ NNPDF2.3 QED  $\rightarrow$  NNPDF3.0 QED
  - ❖ **fit to data**
- ❖ CT14 QED, CT14 QED\_inc [see D. Stump]
- ❖ Harland-Lang, Khoze, Ryskin 2016 [see L. H-L]
- ❖ LUXqed 2016: Manohar, Nason, Salam, Zanderighi
  - ❖ **use ep scattering and construct a hypothetical model for neutral lepton**

ratio to LUXqed

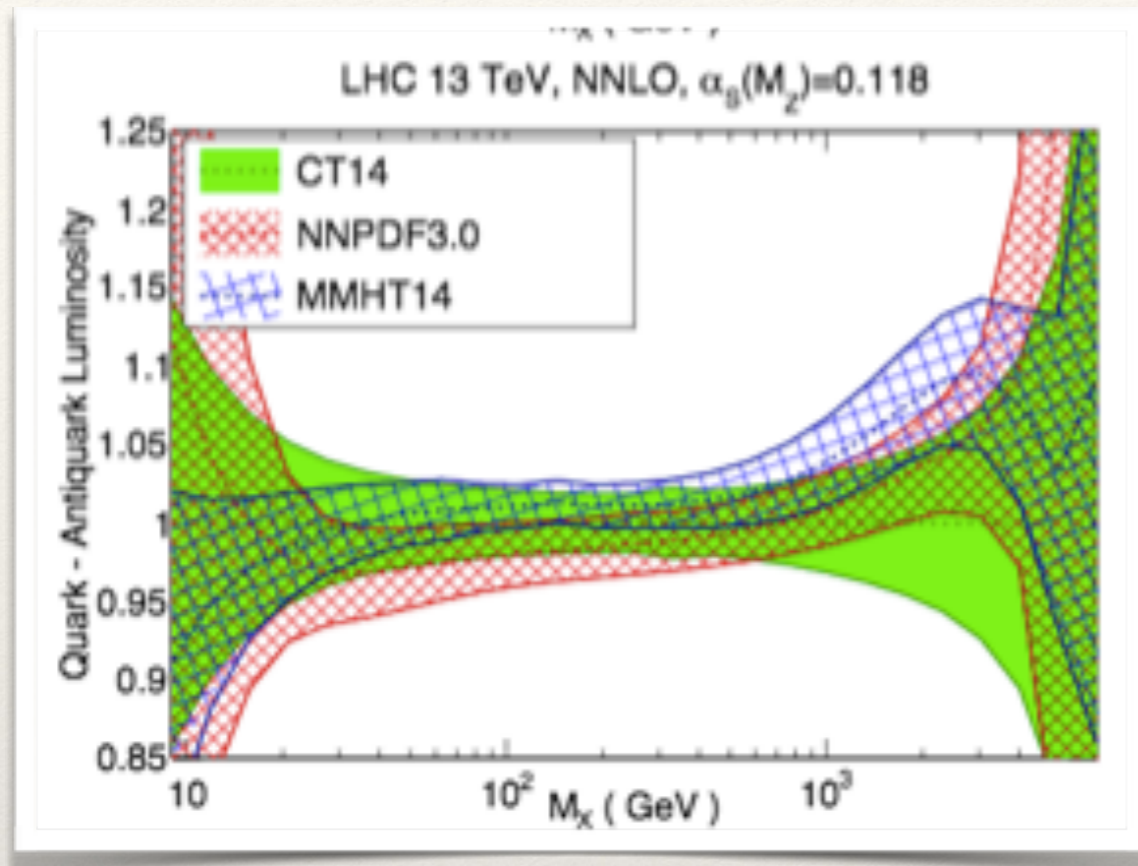


G. Salam

$\rightarrow$  interesting to confront these models with data

# Search for new physics at high scales:

[arXiv:1410.6810v2]



For masses  $>1$  TeV, PDF uncertainties increase to  $> 15\%$

—> can we then distinguish a possible signal?

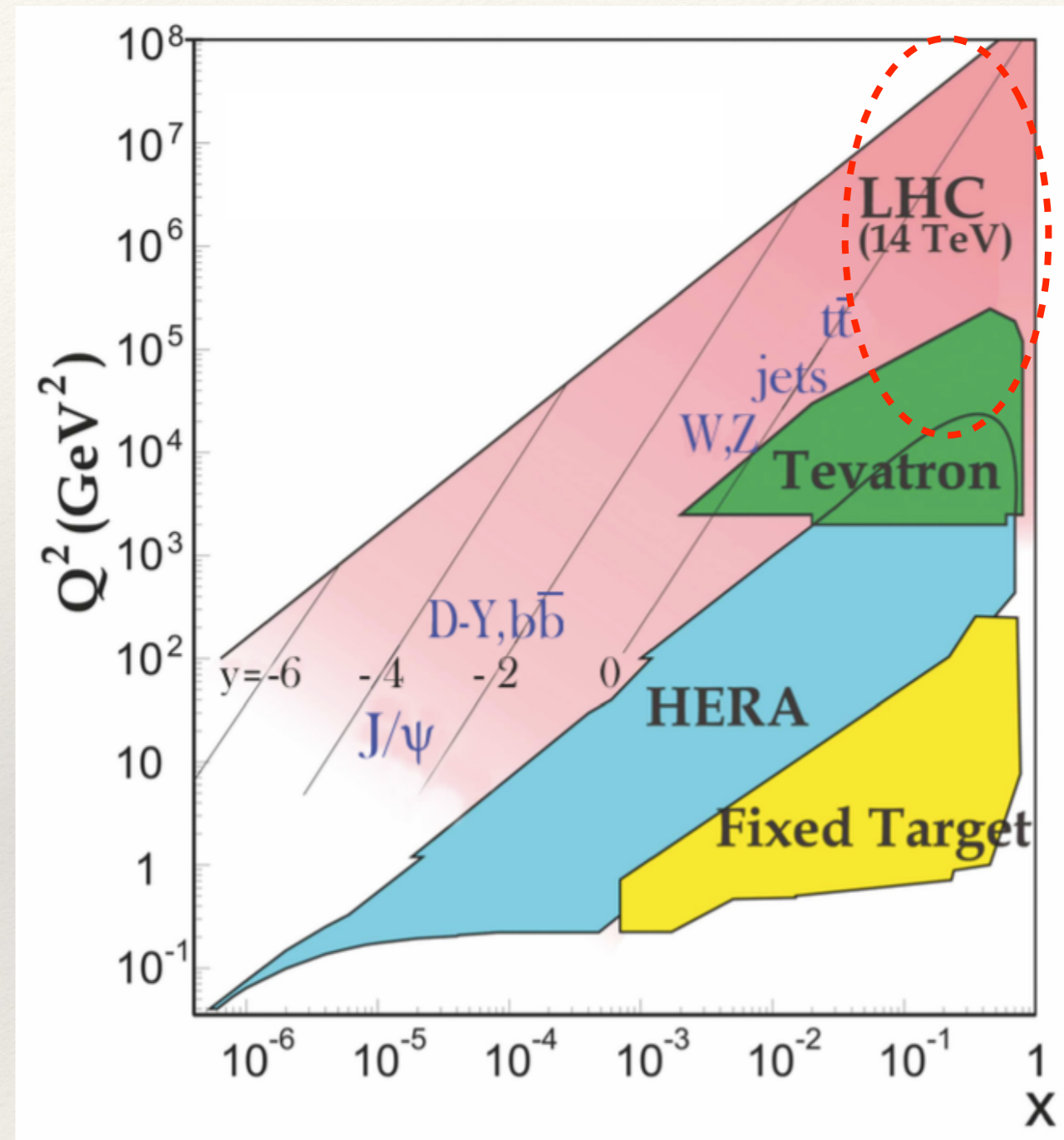
—> scale uncertainties (missing HO) vs PDFs

PDFs then drive the main theory uncertainty

how to improve?

LHC data vs state-of-the-art theory (@NNLO)

- ❖  $t\bar{t}$  can be interesting channel
- ❖ high mass DY can extend to high lever arm reach
- ❖ jet data

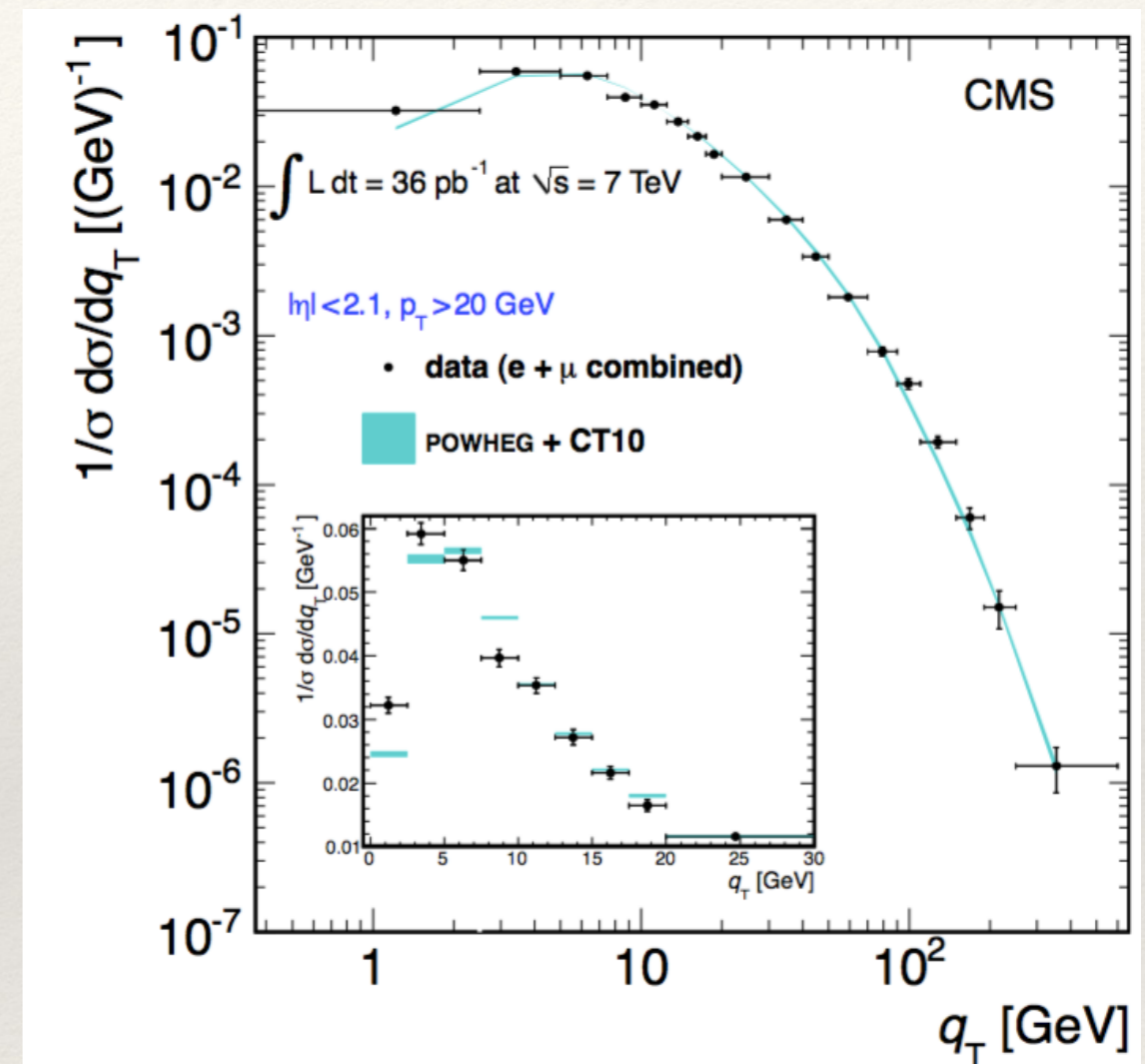


high mass  $\longleftrightarrow$  high  $x$

# Fixed order calculations vs Resummed or + PS

- ❖ Fixed order calculations don't always work and in order to improve the quality of PDF fits in small/high  $x$  regions there have been efforts in providing PDFs consistent with Resummed Computations

- ❖ high- $q_T$  region
  - ❖ it is expected to be described by f.o.
- ❖ at low and peak  $q_T$ 
  - ❖ QCD radiation not described by truncated pQCD
  - ❖ it requires methods to resum arbitrary many parton emissions



There are different approaches to address the failure of f.o. calculations

# TMDs

- ❖ Fixed order calculations don't always work and in order to improve the quality of PDF fits in small/high  $x$  regions there have been efforts in providing PDFs consistent with Resummed Computations

MC simulation combine f.o. partonic calculations with PS and hadronisation  
—> need reshuffling of kinematic variables after PS generations required by energy-momentum conservation

generalisation of QCD factorisation where now the explicit dependence on transverse momentum and polarisations —> TMDs  
they obey the evolution equations which generalise the ordinary RGE of collinear PDFs  
—> allows resummations of large logs ( $M/q_T$ ) to all orders in alphas

New approach to solve coupled gluon and quark DGLAP evolution equation for Monte Carlos:

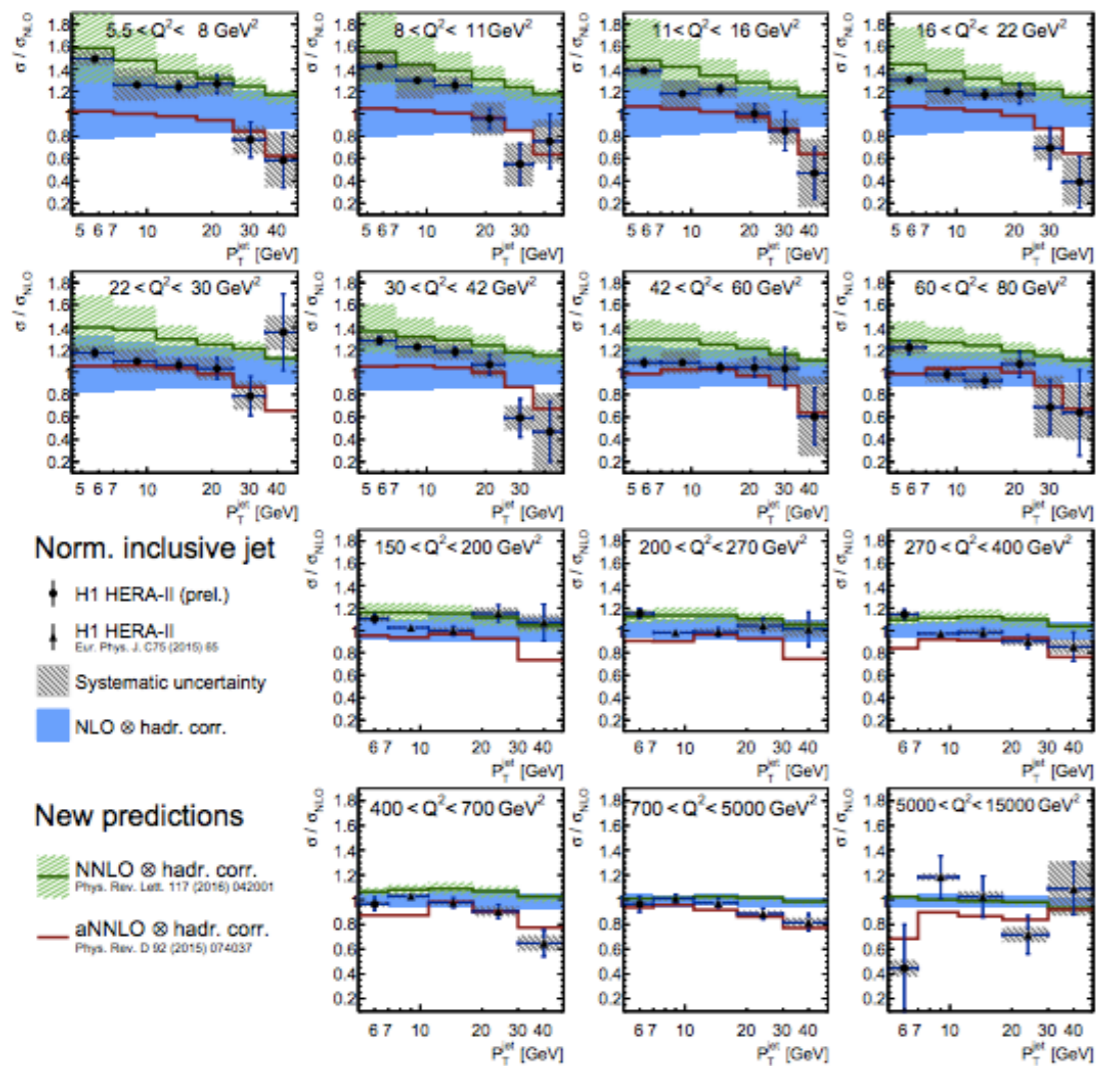
## Advantages:

- ▶ a full TMD pdf evolution including gluon, sea and valence quarks over the full range in  $x$  and  $Q^2$  with the  $k_T$  dependence in the whole kinematically available range (not limited to the small  $k_T$ ),
- ▶ reproduce semi-analytical solution (results consistent with QCDNum), [using TMDs in xFitter]
- ▶ direct usage in PS matched calculation.

credit: H. Jung, F. Hautmann, A. Lelek

# First NNLO for jets @ H1, HERA

H1prelim-16-062



Predictions	NLO	aNNLO	NNLO
Jet cross sections			
Program	nlojet++	JetViP	NNLOJET
pQCD order	NLO [8]	approximate NNLO [12]	NNLO [15]
Calculation detail	Dipole subtraction	NLO plus NNLO contributions from unified threshold resummation formalism	Antenna subtraction
NC DIS cross sections			
Program	QCDNUM	APFEL	APFEL
Heavy quark scheme	ZM-VFNS	FONLL-C	FONLL-C
Order	NLO	NNLO	NNLO
PDF	NNPDF3.0_NLO	NNPDF3.0_NNLO	NNPDF3.0_NNLO
$\alpha_s(M_Z)$	0.118	0.118	0.118
Hadronisation corrections		Djangoh and Rapgap	
Available for			
Normalised inclusive jet	✓	✓	✓
Normalised dijet	✓		✓
Normalised trijet	✓		

- ❖ This opens up a new avenue for PDF fits
  - a boost to re-analyse Tevatron and LHC jets !

# Expectations from LHC data

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## ❖ **Gluon:**

- ❖ Inclusive jets, dijets, trijets → medium / large x
- ❖ Isolated photon and photon+jets → medium / large x
- ❖ ttbar production → large x
- ❖ Zpt spectrum → small / medium x

## ❖ **Quarks:**

- ❖ W and Z rapidity spectra → medium x
- ❖ High pT W+jets → medium / large x
- ❖ Low mass and high mass DY → small / large x
- ❖ W+c rapidity spectrum → strange at medium x
- ❖ single top differential → medium / high x

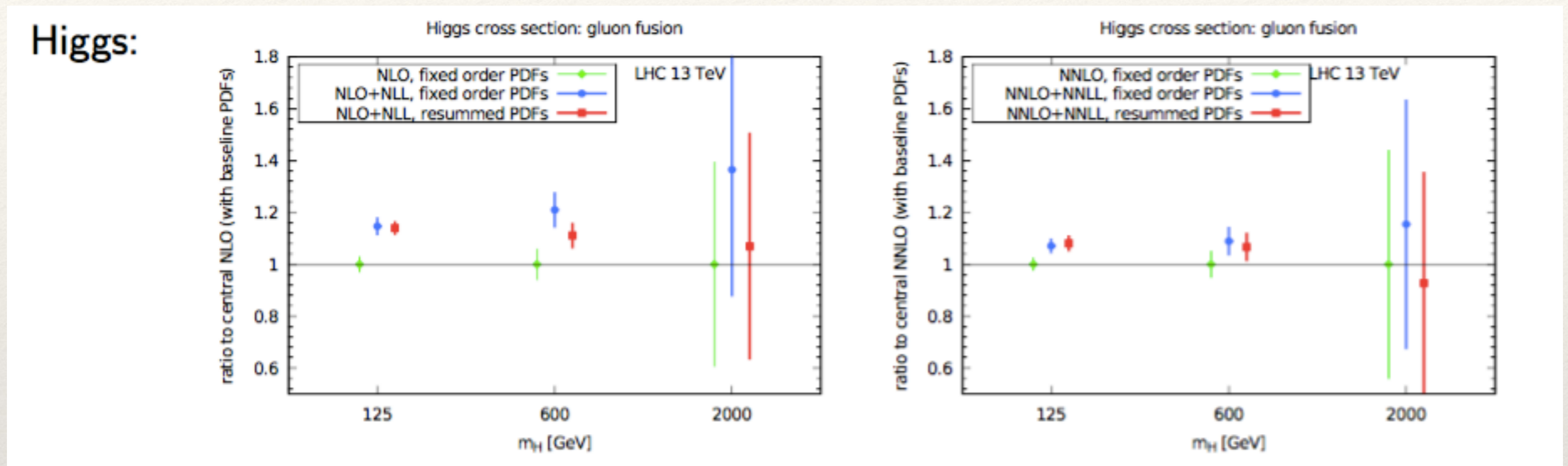
## ❖ **Photon:**

- ❖ WW production
- ❖ High Mass DY



# PDFs with resummed calculations

- ❖ Impact of the resummed PDFs vs fixed order PDFs:



- ❖ Tools for fitting development:

- ❖ HELL: High-Energy Large Logarithms interfaced to APFEL

- ❖ based on the ABF approach for resummation
- ❖ which delivers resummed splitting functions and coefficient functions
- ❖ Therefore could be used for fitting using resummed evolution together with the resummed coefficient functions