# OPENQCDRAD

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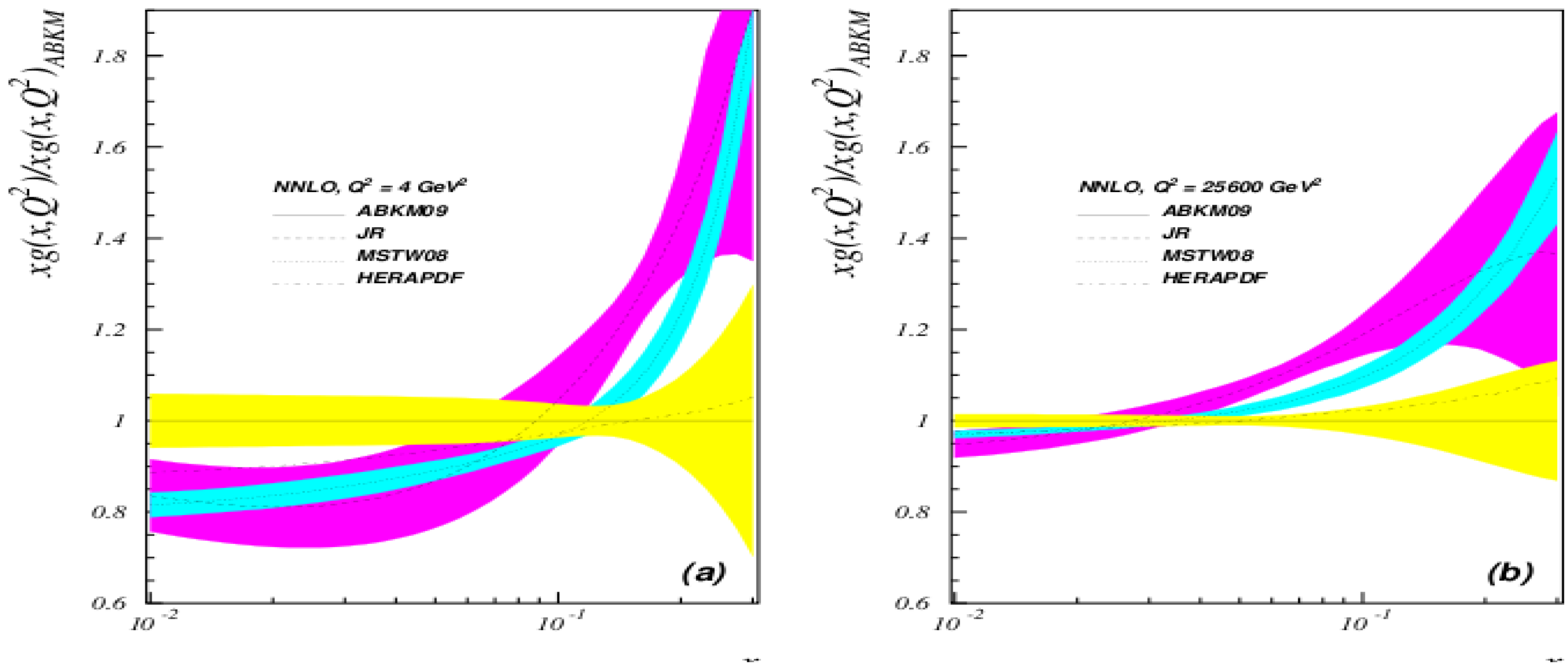
- Motivation
- Theoretical footing
- Structure of the code
- Basic variables and functions
- Examples

DESY, 23 Oct 2012

# PDF benchmarking




**sa, Blümlein, JImenez-Delgado, Moch, Reya PLB 697, 127 (2011)**

The PDFs are different despite agreement with the data in each fit is good → different data sets and different theoretical assumptions

Open code: access to the theoretical details of ABM fits

Interface to other published PDFs

External use: ultimate theoretical accuracy for the DIS

# Theoretical accuracy (3-flavour scheme)

**Massless coefficients:** neutral current (γ, Z, γ-Z), up to NNLO

charged current, up to NNLO

**Massive coefficients:** neutral current (γ) up to NLO

approx. NNLO

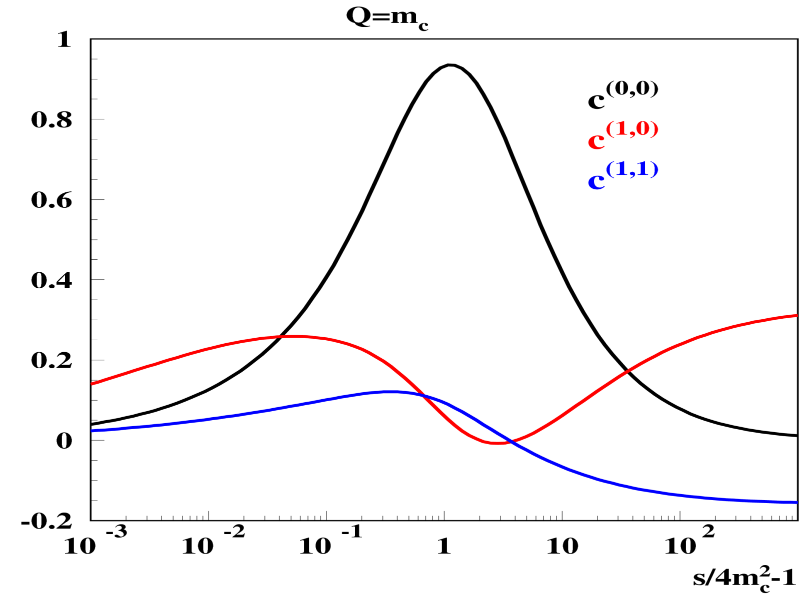
charged current up to NLO

**Massive OMEs:** up to NLO

# Threshold approximation in the DIS

$$x^{-1}F_2^c(x,Q^2,m^2) = \frac{\alpha_s\, e_q^2}{\pi^2} \sum_{i=q,\bar{q},g} \int_0^{\eta_{max}} d\eta\; f_i\left(z(\eta),\mu^2\right)\; c_{i,k}\left(\eta,\xi,\mu^2\right)$$

- At small $x$ and small $Q$ the main contribution comes from $\eta<1$ due to the gluon distribution shape (threshold production)
- The large logs ~ $\ln^n(\beta)$ can be resummed in all orders, this gives a good approximation to the exact NNLO expression at small $\beta$ with the tower of large logs

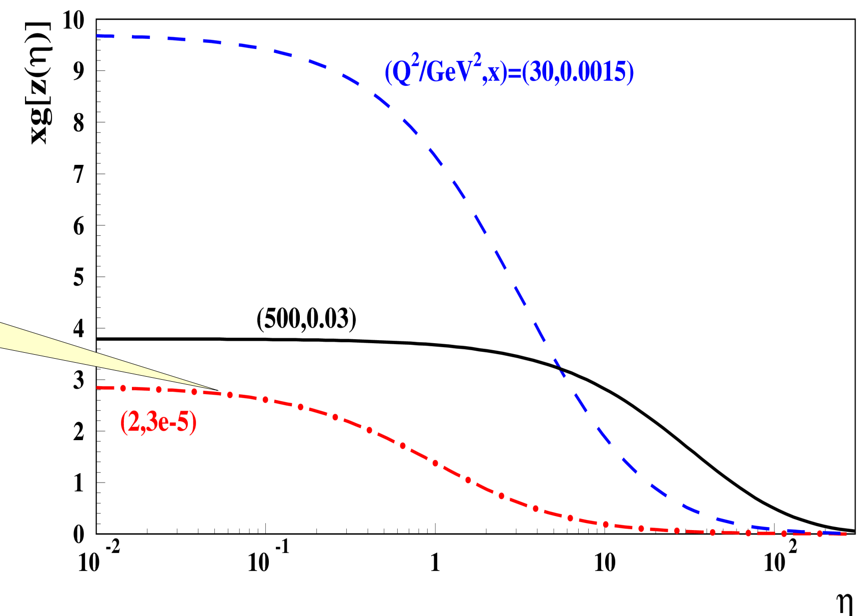



**Laenen, Moch PRD 59, 034027 (1999)**

**sa, Moch PLB 672, 166 (2009)**

*The threshold approximation works in a best way at small Q and x*

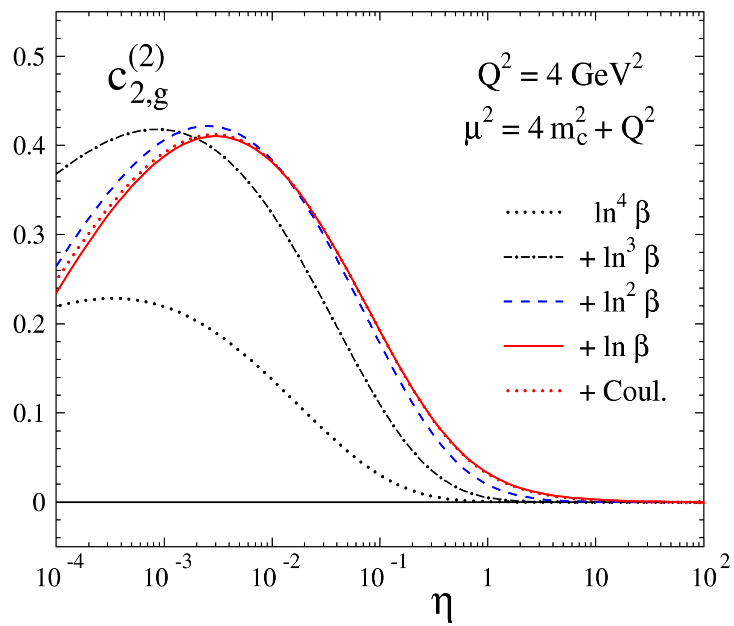
**Vogt hep-ph/9601352**

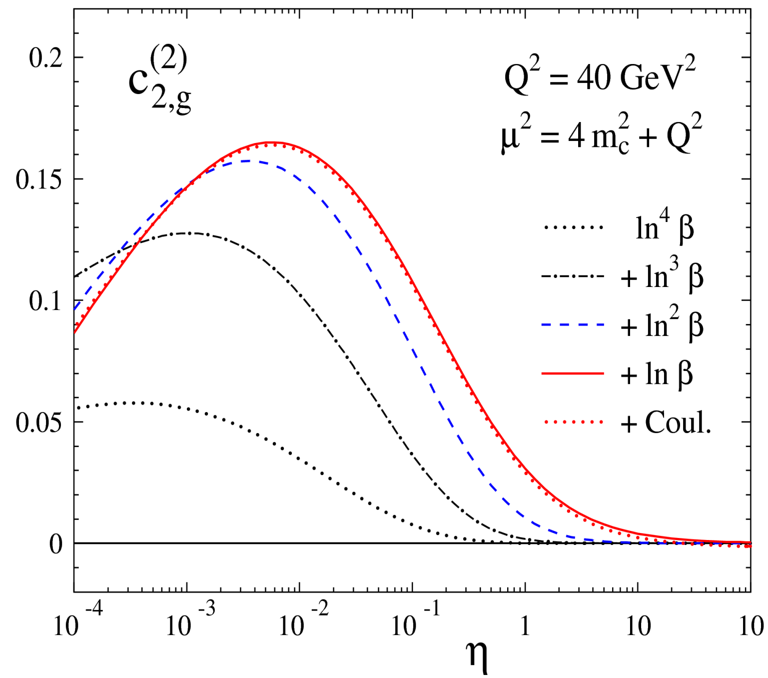



$\eta = s/4m^2 - 1$ – distance to the threshold

$\beta = \sqrt{1-4m^2/s}$ – quark velocity

# Progress in the threshold calculations

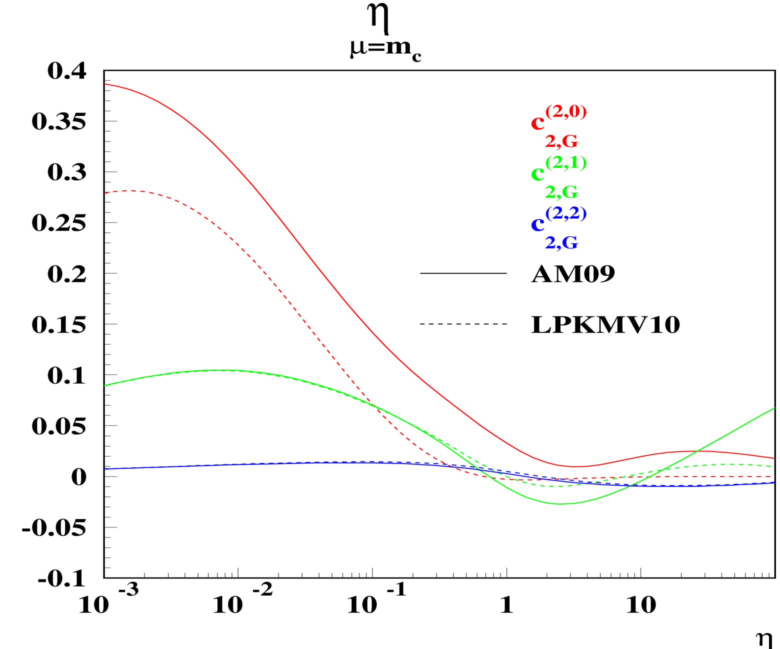



- The first log, Coulomb and linear terms have been recently added → $F_2^c$ gets somewhat smaller at small Q and somewhat bigger at large Q

  **Lo Presti, Kawamura, Moch, Vogt [hep-ph 1008.0951]**

  **Kawamura, Lo Presti, Moch, Vogt NPB 864, 399 (2012)**



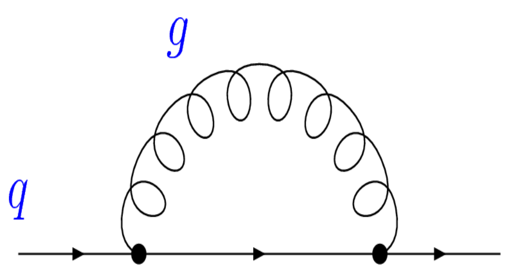
# Pole mass definition

The pole mass is defined as a the QCD Lagrangian parameter and is commonly used in the QCD calculations

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \sum_{\text{flavors}} \bar{q} \left( i \not{D} - m_q \right) q$$

Pole mass is defined for the free (unobserved) quarks

$$\not{p} - m_q - \Sigma(p, m_q) \Big|_{p^2 = m_q^2}$$

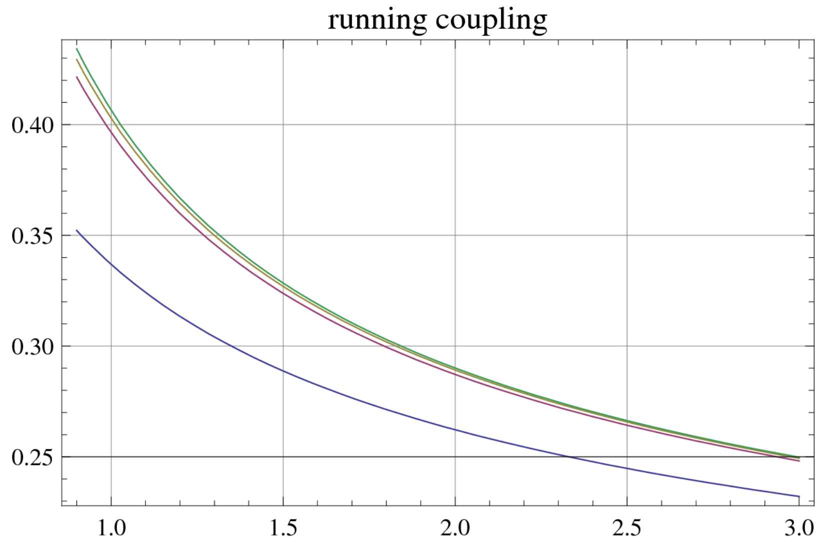


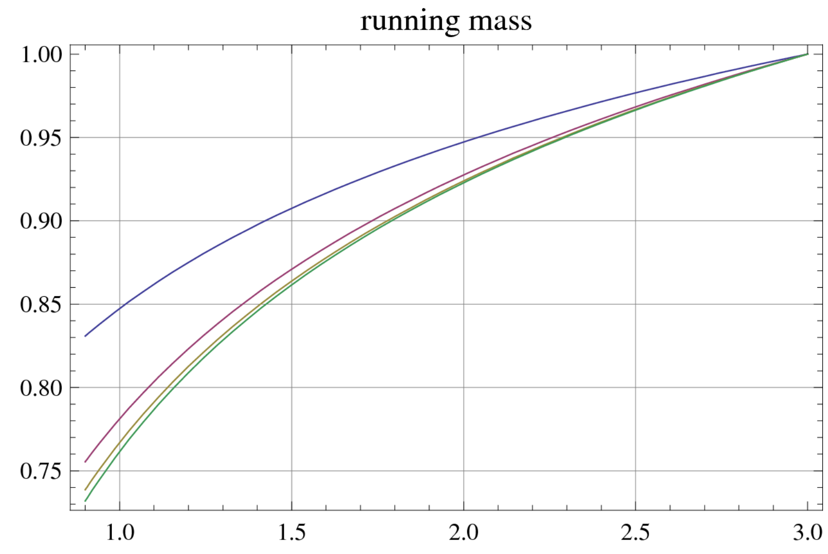

The quantum corrections due to the self-energy loop integrals receive contribution down to scale of $O(\Lambda_{QCD})$ → sensitivity to the high order corrections, particularly at the production threshold

# Running quark mass

The renormgroup equation for mass is similar to one for the coupling constant

$$\mu^2 \frac{d}{d\mu^2}\alpha_s(\mu) = \beta(\alpha_s) \qquad \mu^2 \frac{d}{d\mu^2} m(\mu) = \gamma(\alpha_s) m(\mu)$$




The corrections up to 4-loops are known

van Ritbergen, Vermaseren, Larin PLB 400, 379 (1997)

Chetyrkin PLB 404, 161 (1997)

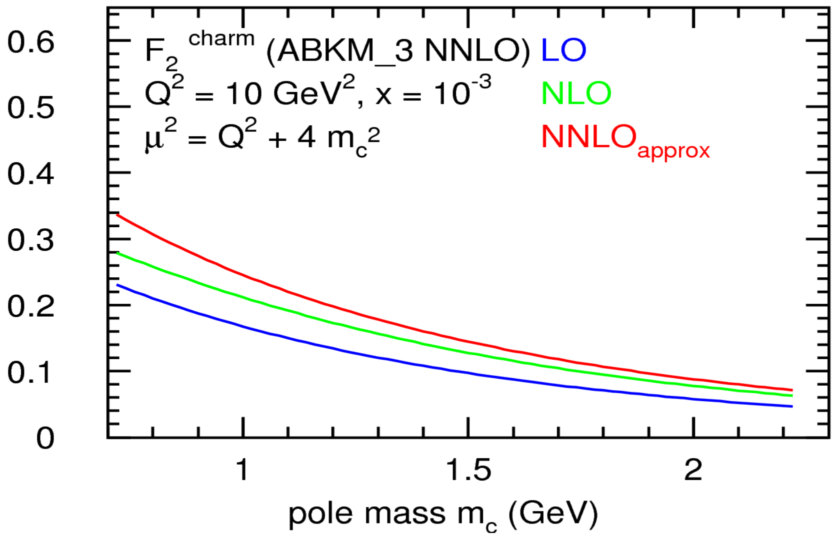
Vermaseren, Larin, van Ritbergen PLB 405, 327 (1997)

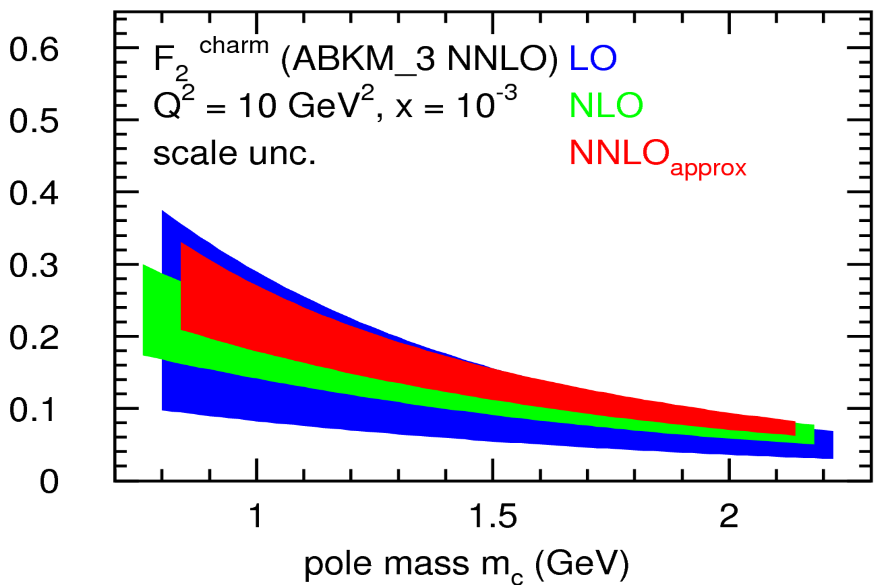
The choice of $\mu_R = m_c$ is close to the hard scattering data kinematic → better perturbative convergence and reduced scale dependence

- The ttbar production in hadronic collisions Laengenfeld, Moch, Uwer PRD 80, 054009 (2009)

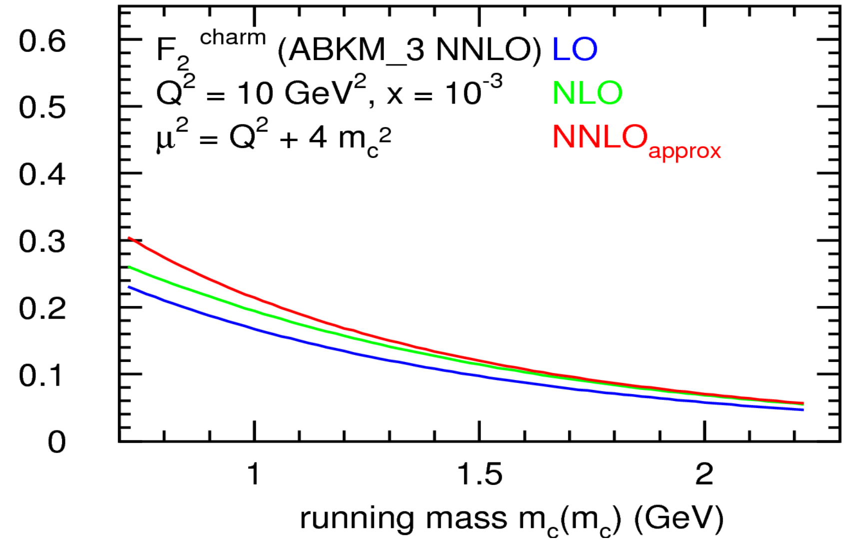
# DIS SFs with the running mass definition

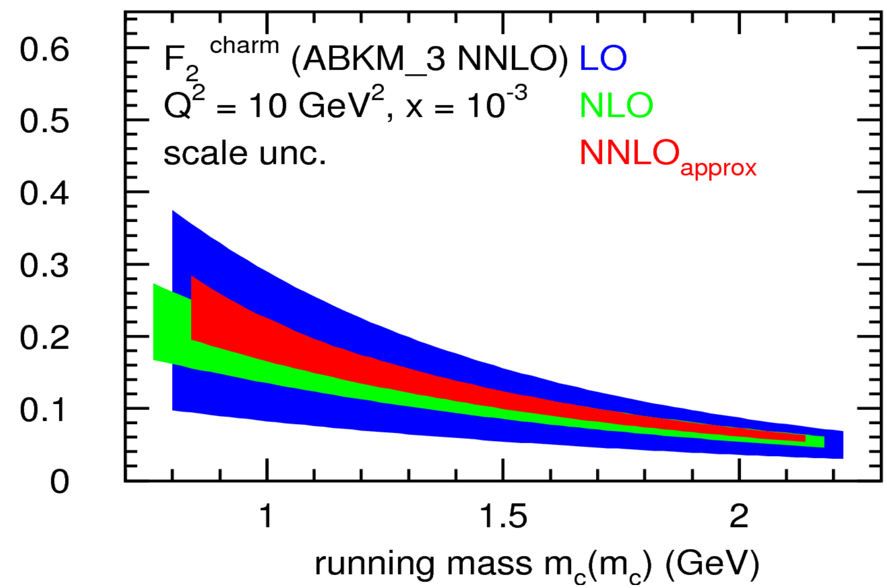
## Pole mass



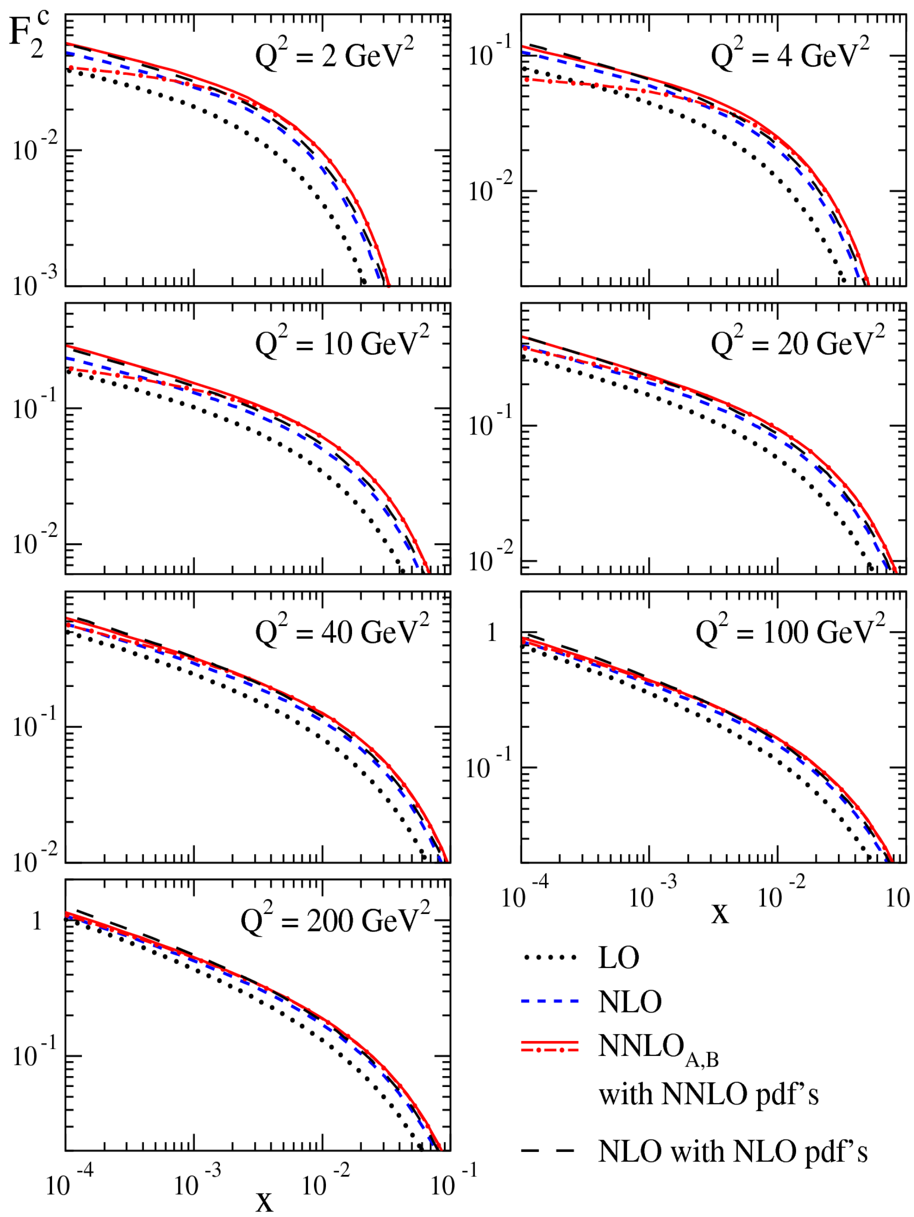

## Running mass




**sa, Moch PLB 699, 345 (2011)**

# State-of-art massive NNLO coefficients




Kawamura, Lo Presti, Moch, Vogt NPB 864, 399 (2012)

- The NNLO log terms are known due to the recursive relations
- The constant NNLO term stem from:
  - the threshold resummation terms including the Coulomb one
  - high-energy asymptotics obtained with the small-x resummation technique

    Catani, Ciafaloni, Hautmann NPB 366, 135 (1991)

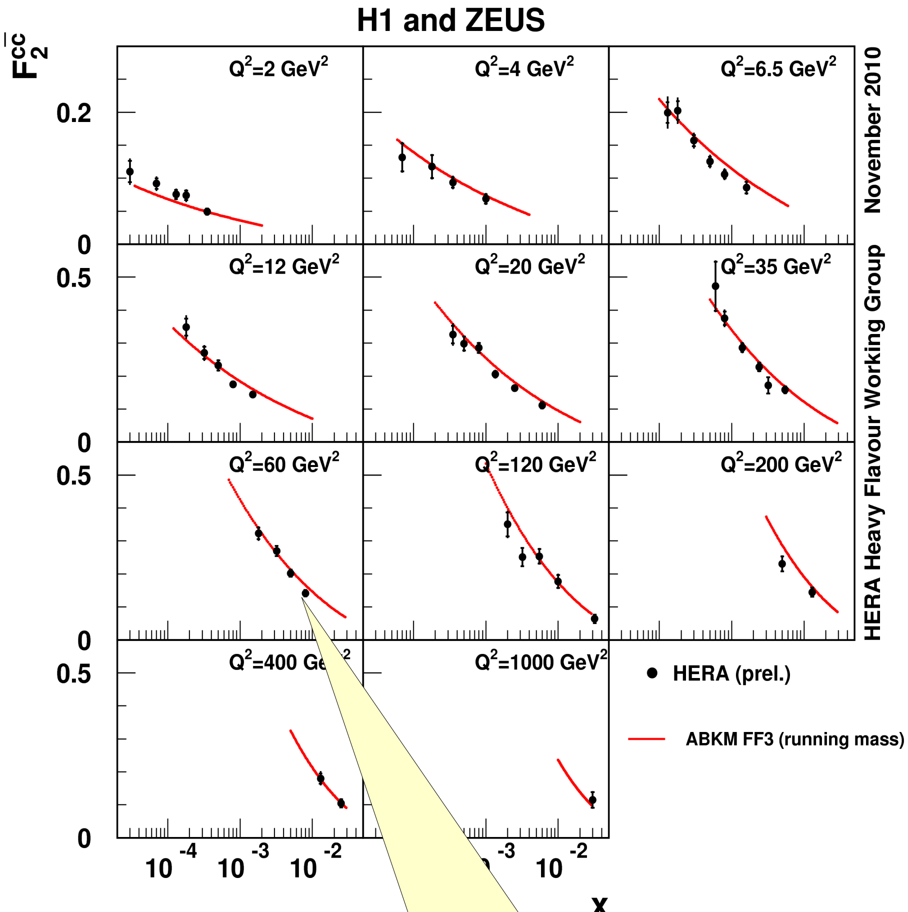
  - available NNLO Mellin moments for the massive OMEs

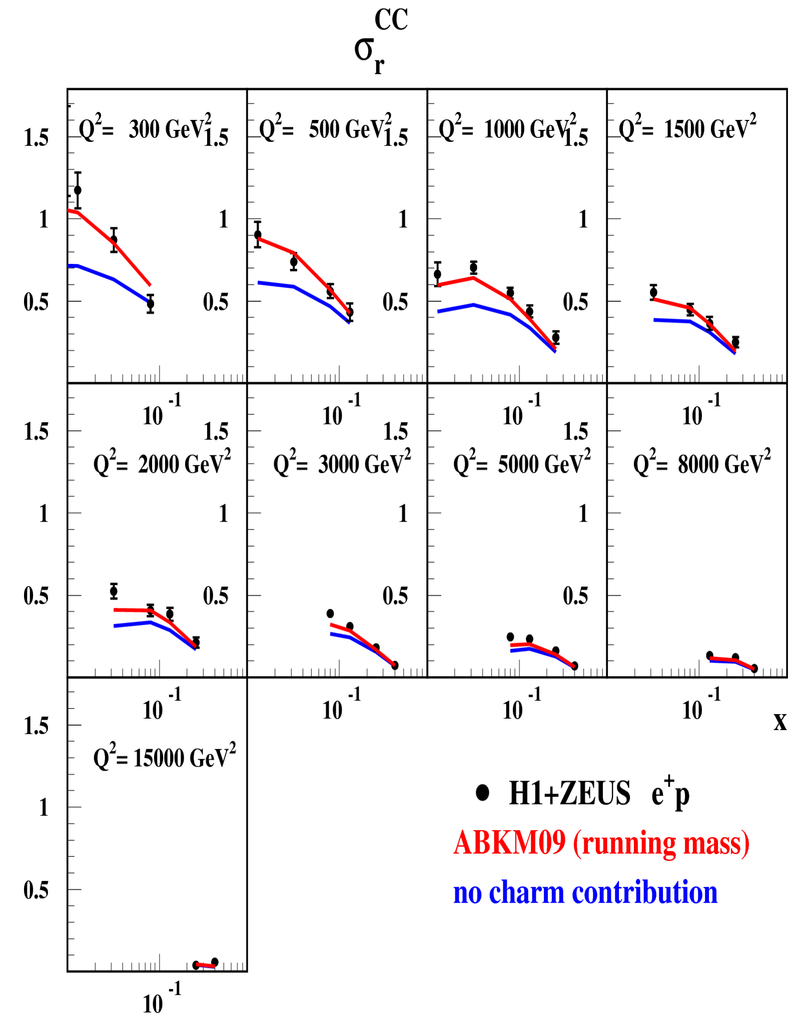
    Ablinger at al. NPB 844, 26 (2011)

    Bierenbaum, Blümlein, Klein NPB 829, 417 (2009)
- The uncertainty in the NNLO coefficients is due to matching of the threshold corrections with the high-energy limit → two options for the coefficients are provided
- Further improvement should come from additional Mellin moments

Blümlein at al. in progress

# FFNS versus HERA data

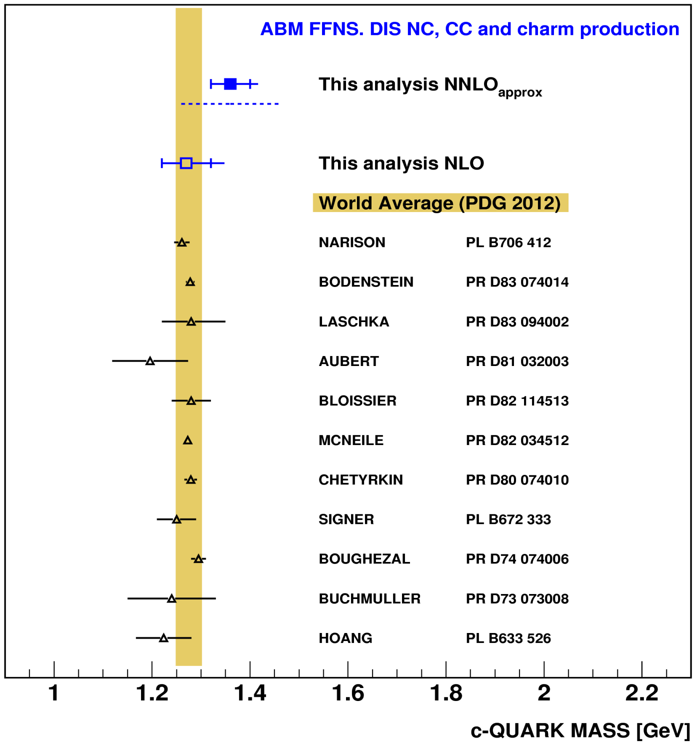



No need of the resummation

The NNLO FFNS ***predictions*** based on the running mass definition are in a good agreement with the recent HERA data

# Heavy-quark mass definition




sa, Daum, Lipka, Moch hep-ph/1209.0436

In contrast, the values of pole mass $m_c$ used by different groups and preferred by the PDF fits are systematically lower than the PDG value

| | MSTW | NNPDF | JR | CTEQ | PDG |
|---|---|---|---|---|---|
| $m_c$(GeV) | 1.40 | $\sqrt{2}$ | 1.3 | 1.3 | 1.66 |

| $m_c$ (GeV) | $\chi^2_{\text{global}}$ (2615 pts.) | $\chi^2_{F_2^c}$ (83 pts.) | $\alpha_S(M_Z^2)$ |
|---|---|---|---|
| 1.1 | 2498 | 113 | 0.1159 |
| 1.2 | 2463 | 88 | 0.1162 |
| 1.26 | 2456 | 82 | 0.1165 |
| 1.3 | 2458 | 82 | 0.1166 |
| **1.4** | 2480 | 95 | 0.1171 |
| 1.5 | 2528 | 126 | 0.1175 |
| 1.6 | 2589 | 167 | 0.1180 |
| 1.7 | 2666 | 217 | 0.1184 |

Martin, Stirling, Thorne, Watt [hep-ph 1007.2624]

From the fit to the H1 charm production data the c-quark running mass values are

$m_c(m_c)$=1.27±0.05(exp.) GeV NLO

1.36±0.04(exp)±0.1(theo) GeV NNLO

in agreement with PDG

# Benchmark of the DIS with the 3-flavor PDFs

The DIS data play crucial role for the small-x PDFs however they are analyzed using different schemes: FFNS and various GMVFN prescriptions

Matching of the 3-, 4-, and 5-flavour PDFs is unique up to the matching point

**Buza, Matounine, Smith, van Neerven EPJC 1, 301 (1998)**

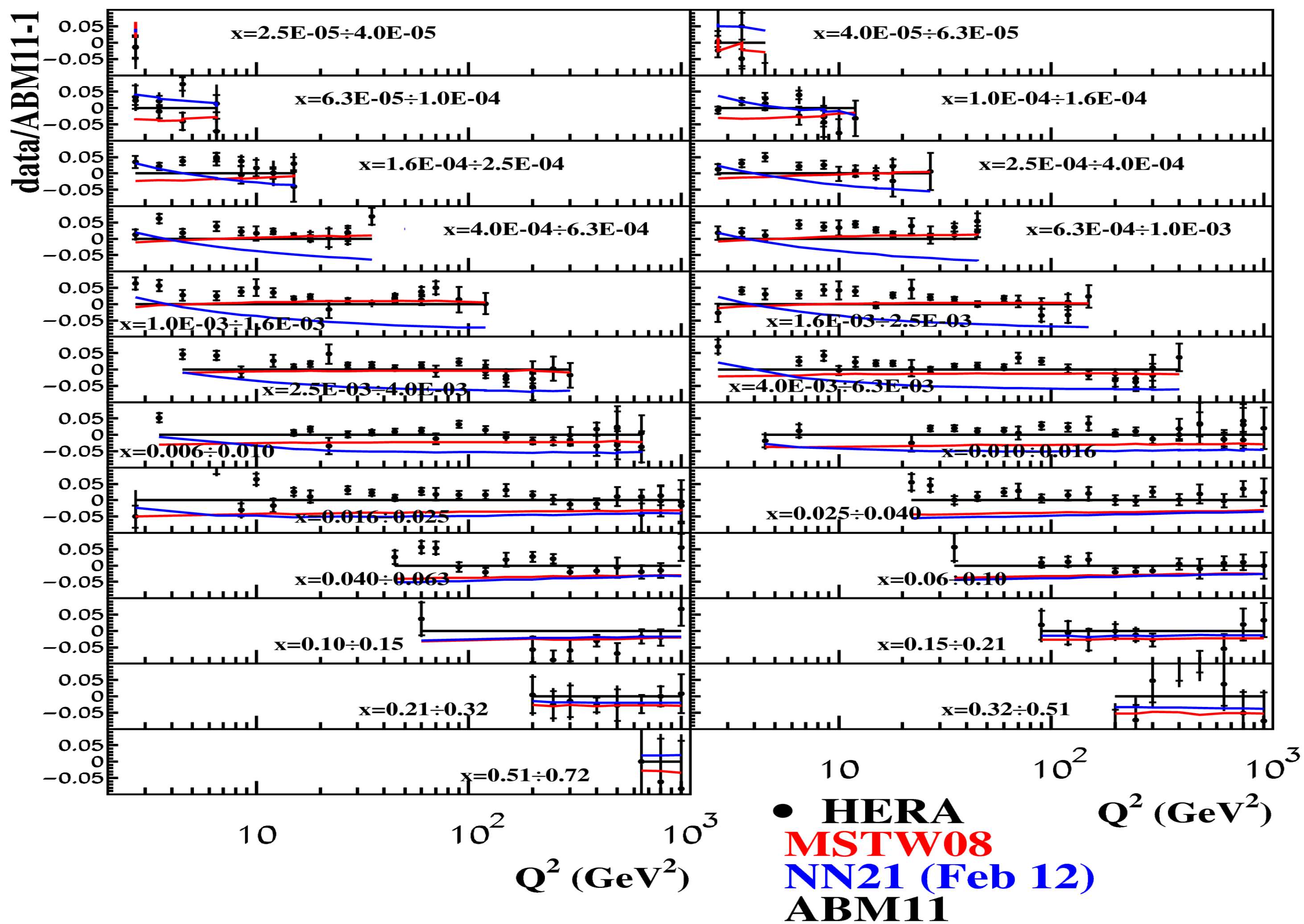
The 3-flavor PDFs are often provided even the fit is based on the GMVFNS and can be easily generated otherwise

- Convolution with the FFNS coefficient must reproduce the FFNS results at small scales once a GMVFNS should tend to FFNS
  - For the fixed-target data the heavy-quark contribution is marginal and the scheme choice is unimportant
  - At large Q the data may overshoot the predictions due to impact of big logs

*Account of the massive NNLO corrections is crucial*

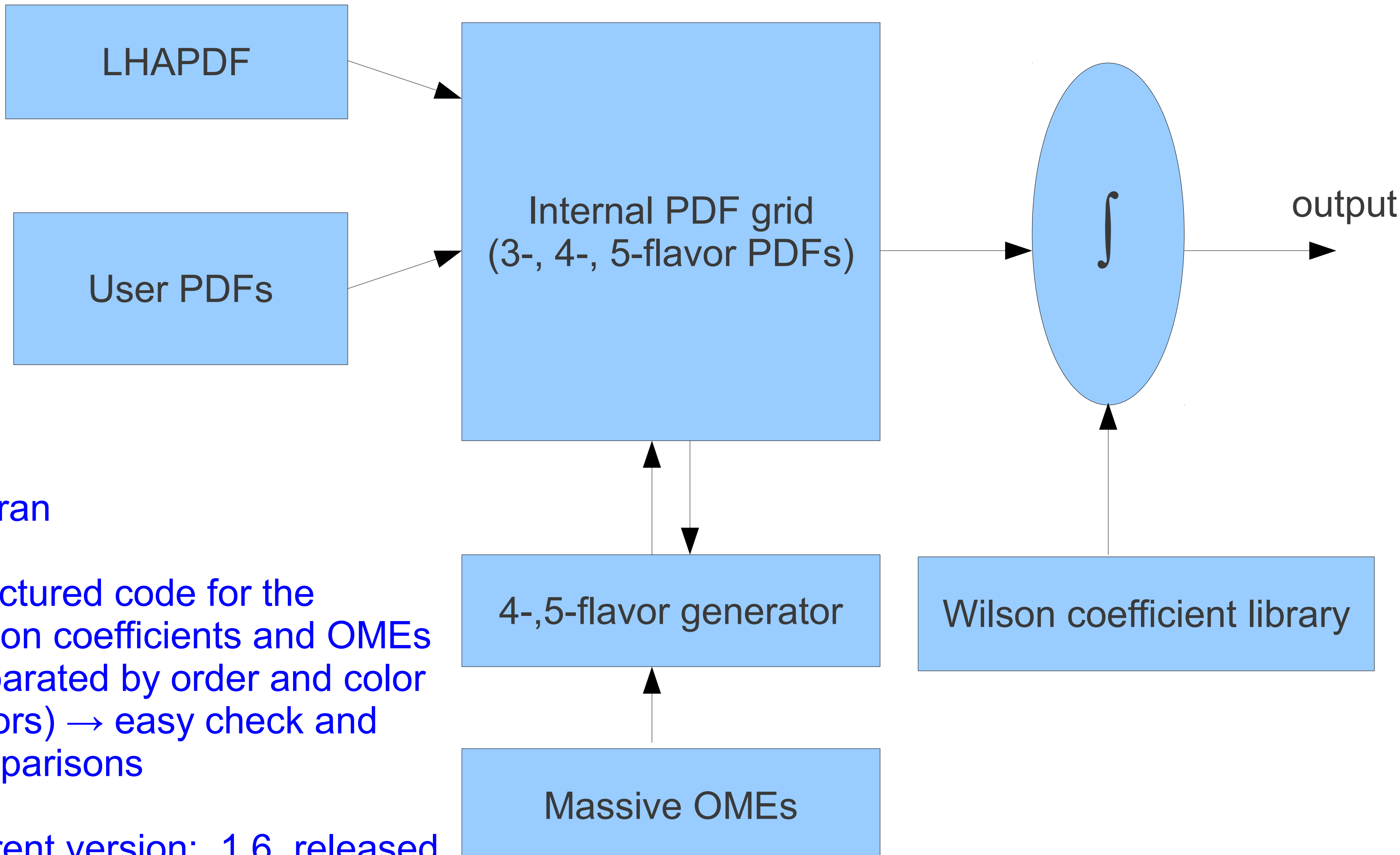
# OPENQCDRAD benchmark for the HERA data

**H1 and ZEUS JHEP 1001, 109 (2010)**




The data clearly discriminate different PDFs; the differences can be localized and traced back to the particular features of the PDF fit ansatz, presumably difference in the GMVFNS prescriptions

# Logical structure




Fortran

Structured code for the Wilson coefficients and OMEs (separated by order and color factors) → easy check and comparisons

Current version: 1.6, released Oct'12

www-zeuthen.desy.de/~alekhin/OPENQCDRAD

# Front-end routines

Initialization:

Initgridconst – initialization of constants, the PDF grid spacing, and generation of interpolation tables for the Involved expressions

Pdffillgrid – fills internal PDF grid

Light partons:

f2qcd(nb,nt,ni,xb,q2)
flqcd(nb,nt,ni,xb,q2)
f3qcd(nb,nt,ni,xb,q2)

Heavy quarks in FFNS:

NC: f2charm_ffn(xb,q2,nq)
flcharm_ffn(xb,q2,nq)

CC: f2nucharm(nb,nt,ni,xb,q2,nq)
ftnucharm(nb,nt,ni,xb,q2,nq)
f3nucharm(nb,nt,ni,xb,q2,nq)

Heavy quarks in GMVFZNS/BMSN

f2h_bmsn(ni,nb,nt,xb,q2,nq)

nb – beam type (electron, neutrino)
nt – target type (proton, neutron)
ni – exchange boson type (γ, Z, W, γ-Z)
nq – heavy quark type (c, b)

# Steering parameters

PDF selection

kschemepdf – 3,-,4-, and 5-flavor PDFs will be stored by PDFFILLGRID for kschemepdf=0,1,2, respectively
kordpdf – LO, NLO, and NNLO PDFs will be stored for kordpdf=0,1,2, respectively
kpdfset – selects LHAPDF member of the PDF uncertainty family

Theoretical accuracy (Wilson coefficient order)

kordf2, kordf3 – 0: LO, 1: NLO, 2: NNLO for the light-parton F2 and F3
kordfl – 1: LO, 2: NLO, 3: NNLO for the light-parton FL
kordhq – 0: LO, 1: NLO, 2: NNLO for the heavy-quark SFs

Heavy-quark definitions

msbarm – .false. : pole-mass, .true. : running mass
hqnons – .false. / .true. : non-singlet term included/excluded
hqscale1
hqscale2 – factorization scale setting

more details in .../doc/manual.pdf

# File structure

..../qcdlib – source code of the Wilson coefficients, OMEs, and convolution routines. editing is not recommended

…./user – template for the user interface to PDFs, should be properly edited before the code compilation

…./dis – various examples of calculating the DIS SFs, should be used as templates for the user applications

…./pdfs – various examples of calling the PDFs, should be used for checking interface to LHAPDF

…/doc – selected list of the steering parameters

…../m4/ – autoconf macros, can be used to set proper system environment for the user applications (compiler options, libraries settting, etc.)

# Compilation and running

Compilation:

autoreconf
configure
make PDFSET=ABM11

the PDF set is selected at compilation
(options: CT10, HERAPDF1, JR09
MSTW08, NN21, USER)

→ static library …./qcdlib/libqcdradopen.a (*or make install*)
set of the example codes

Dependencies:

LHAPDF is properly installed:

*lhapdf-config –datadir* should give a path to the PDF grids
*lhapdf-config –libdir* should give a path to the LHAPDF library

configure –with-usercern=/path/to/the/CERN/library if CERN libraries are not in /cern/pro/lib

Running:

make run BENCH=name-of-the-template-code in …/dis or …/pdfs
to run examples of using the code

more details in README

# List of examples

-- The neutral-current inclusive DIS cross sections for the kinematics of NuTeV experiment

-- The charged-current structure functions F_2,L,3 for the kinematics of combined H1 and ZEUS data and calculated in the running mass definition

-- The neutral-current semi-inclusive DIS structure functions F_2,L^hh for the kinematics of combined H1 and ZEUS data and calculated in the approximate NNLO for the running mass definition

-- The neutral-current semi-inclusive DIS structure functions F_2,L^hh calculated in the NLO and approximate NNLO for the running mass and pole mass definitions; the same for the charged-current semi-inclusive structure functions F_2,3,T^cc calculated in the NLO

-- The semi-inclusive F_2,L^cc and inclusive DIS structure function F_2,L calculated in the fixed-flavor-number scheme and Buza-Matiounine-Smith-van Neerven prescription of the general-mass variable flavor number scheme for the planned EIC kinematics in the NNLO approximation:

```
      include 'CONSTCOM.'
      INCLUDE 'PDFCOM.'
      call initgridconst
!  Set up the 3-flavour NNLO PDFs and fill the 3-flavour PDF grid
      kschemepdf=0
      kordpdf=2
      call pdffillgrid
!  Set the factorization scale as sqrt(Q2*hqscale1 + 4m^2*hqscale2) for the
!  pair heavy-quark production and as sqrt(Q2*hqscale1 + m^2*hqscale2) for the
!  single heavy-quark production
      hqscale1=1d0
      hqscale2=1d0
!
      xb=1d-3
      q2=10d0
      kordhq=2                              !  NNLO
      msbarm=.true.                         ! running-mass definition
      rmass(8)=1.27                         ! value of the c-quark mass
      a1=flcharm_ffn(xb,q2,8)
      a2=f2charm_ffn(xb,q2,8)
  ……………………………………………………
```

```
export LHAPATH
export GRIDS
run:
	./$(BENCH)
noinst_PROGRAMS = MSBAR
MSBAR_SOURCES = msbar.F
MSBAR_DEPENDENCIES = $(top_builddir)/qcdlib/libqcdradopen.a
```

# Outlook

- Bookkeeping of the available benchmark plots on a public site
- More detailed description (preparing manual?)
- Interface to the evolution code:
  - 3-flavor PDFs for all available sets
- Interface to the data files:
  - facilitated comparison to the data for external users