QCDNUM17

Fast QCD evolution and convolution

Michiel Botje
NIKHEF
PO Box 41882 1009DB Amsterdam

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What is QCDNUM ?

- Fortran program that evolves α_s and the parton densities up to NNLO on a grid in x and Q^2
- Possibility to vary renormalisation scale with respect to the factorisation scale
- Convolution of pdfs with a Wilson coefficient in zero mass or in any generalised mass scheme
- Fast, accurate and user friendly

QCDNUM has a long history...

1988	Code by Ouraou and Virchaux (BCDMS)	CRAY vectorized Fortran
1993	NMC adaptation to low x	CRAY vectorized Fortran
1998	QCDNUM16.12 used by ZEUS	Unix Fortran77
2007	NNLO upgrade QCDNUM17	Unix Fortran77
2009	QCDNUM17-beta-05	Unix Fortran77

DGLAP evolution of PDFs

Singlet/gluon evolution

$$q_s = \sum_{i=1}^{n_f} (q_i + \bar{q}_i)$$

$$\frac{\partial}{\partial \ln \mu^2} \begin{pmatrix} q_s \\ g \end{pmatrix} = \begin{pmatrix} P_{qq} & P_{qg} \\ P_{gq} & P_{gg} \end{pmatrix} \otimes \begin{pmatrix} q_s \\ g \end{pmatrix}$$

Non-singlet evolution

$$\frac{\partial q_{ns}}{\partial \ln \mu^2} = P_{ns} \otimes q_{ns}$$

$$q_{ij}^{\pm} = (q_i \pm \bar{q}_i) - (q_j \pm \bar{q}_j)$$

$$q_v = \sum_{i=1}^{n_f} (q_i - \bar{q}_i)$$

	LO	NLO	NNLO
q_{ij}^{+}	P_{qq}	P_{+}	P_{+}
q_{ij}^{-}	P_{qq}	P_{-}	P_{-}
q_v	P_{qq}	P_{-}	P_{v}

QCDNUM uses internally a standard singlet/non-singlet set of basis functions

Singlet or Valence

$$\begin{pmatrix} e_1^{\pm} \\ e_2^{\pm} \\ e_3^{\pm} \\ e_4^{\pm} \\ e_5^{\pm} \\ e_6^{\pm} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & & & & \\ 1 & 1 & -2 & & & \\ 1 & 1 & 1 & -3 & & \\ 1 & 1 & 1 & 1 & -4 & \\ 1 & 1 & 1 & 1 & 1 & -5 \end{pmatrix} \begin{pmatrix} u^{\pm} \\ d^{\pm} \\ s^{\pm} \\ c^{\pm} \\ b^{\pm} \\ t^{\pm} \end{pmatrix}$$

Non-singlet

$$q_i^{\pm} = q_i \pm \bar{q}_i$$

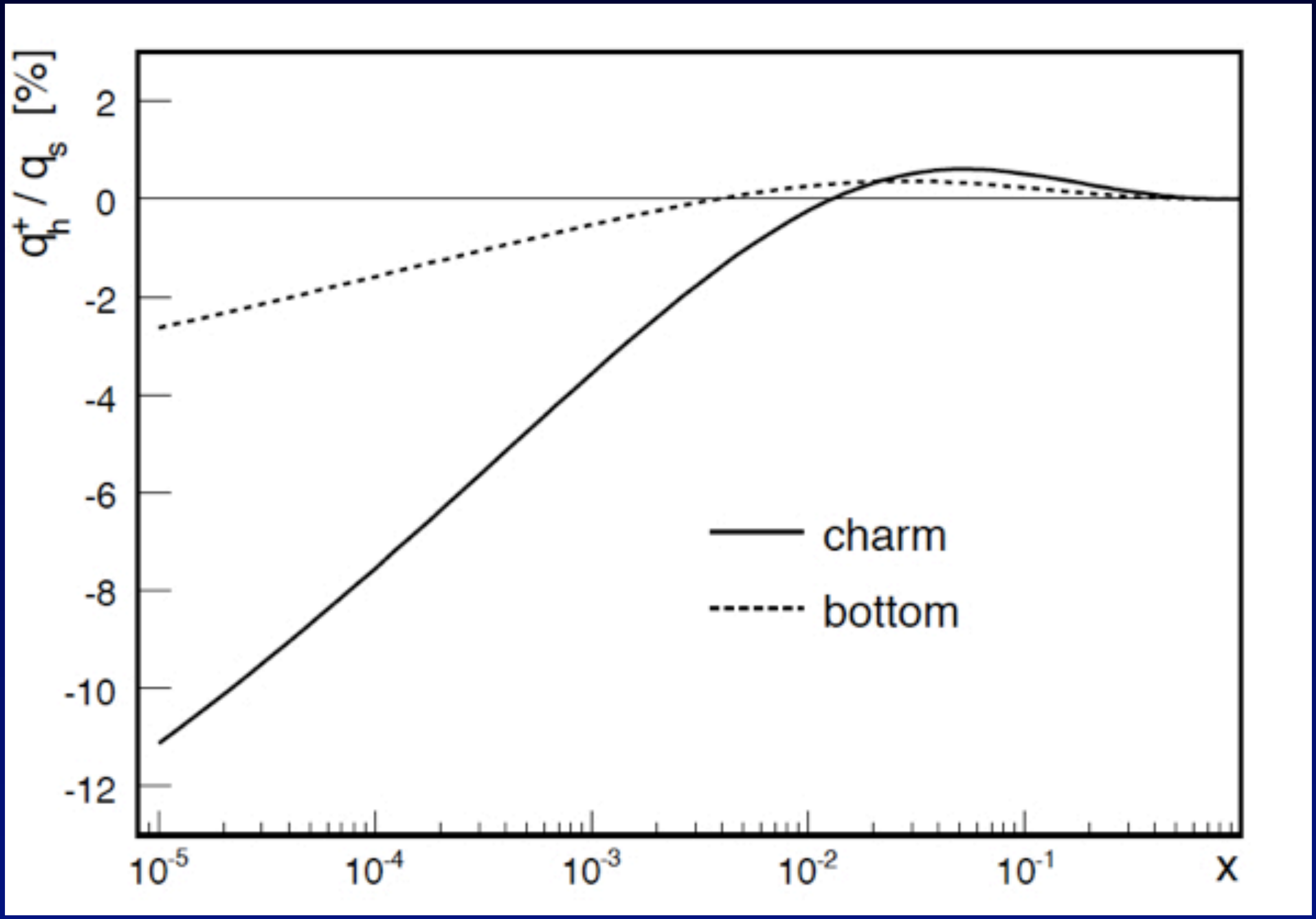
Evolution schemes in QCDNUM

- FFNS: number of active flavours is kept constant $3 < n_f < 6$ for all Q^2
- VFNS: number of flavours changes from n_f to $n_f + 1$ at the thresholds $Q^2_{c,b,t}$
  - Input: gluon + 6 light quark PDFs at $Q^2_0 < Q^2_c$
  - Heavy quark PDFs are generated by the DGLAP evolution equations
  - The PDFs and α_s are continuous at the thresholds in LO and NLO but are discontinuous in NNLO

Chetyrkin et al., PRL 79 (1997) 2184
Buza et al., EPJ C1 (1988) 301

Example: NNLO discontinuity of charm and bottom at their thresholds

- Bottom ~3% of singlet at low x
- Charm ~10%
- PDFs negative below x = 10^{-2}
- No problem since PDFs are not observables



Renormalisation scale dependence

- The strong coupling constant evolves on the renormalisation scale and the PDFs evolve on the factorisation scale
- QCDNUM supports a linear relationship between these two scales

$$\mu_{\mathrm{R}}^2 = a\,\mu_{\mathrm{F}}^2 + b$$

- Allows to study renormalisation scale dependence of PDFs (and STFs, Xsecs)

Numerical method in a nutshell

- Solve DGLAP numerically on a log x-Q^2 grid
- Based on linear and quadratic polynomial spline interpolation on multiple equidistant grids
- Convolution integrals become weighted sums with weights calculated at program initialization
- Evolution step becomes a lower triangular $n \times n$ matrix equation solved by forward substitution
- This matrix roll-up is the only $O(n^2)$ calculation in the whole program, everything else is $O(n)$

☑ QCDNUM is very fast

QCDNUM: compact user interface

```
call QCINIT(6,' ')
call GXMAKE(xmin,1,1,nxin,nx,iosp)
call GQMAKE(qq,wt,2,nqin,nq)
call FILLWT(0,id1,id2,nwords)
call SETORD(3)
call SETALF(as0,r20)
call SETCBT(0,iqc,iqb,iqt)
call EVOLFF(func,def,iq0,eps)
call PDFSXQ(x,q,pdf,0)
```

☑ Full NNLO evolution in 9 lines

QCDNUM: grids and weights

```
call QCINIT(6,' ')
call GXMAKE(xmin,1,1,nxin,nx,iosp)
call GQMAKE(qq,wt,2,nqin,nq)
call FILLWT(0,id1,id2,nwords)
call SETORD(3)
call SETALF(as0,r20)
call SETCBT(0,iqc,iqb,iqt)
call EVOLFF(func,def,iq0,eps)
call PDFSXQ(x,q,pdf,0)
```

- Initialise QCDNUM
- Define x-Q^2 grid and lin/quad interpolation
- Calculate weight tables

QCDNUM: evolution parameters

```
call QCINIT(6,' ')
call GXMAKE(xmin,1,1,nxin,nx,iosp)
call GQMAKE(qq,wt,2,nqin,nq)
call FILLWT(0,id1,id2,nwords)
call SETORD(3)
call SETALF(as0,r20)
call SETCBT(0,iqc,iqb,iqt)
call EVOLFF(func,def,iq0,eps)
call PDFSXQ(x,q,pdf,0)
```

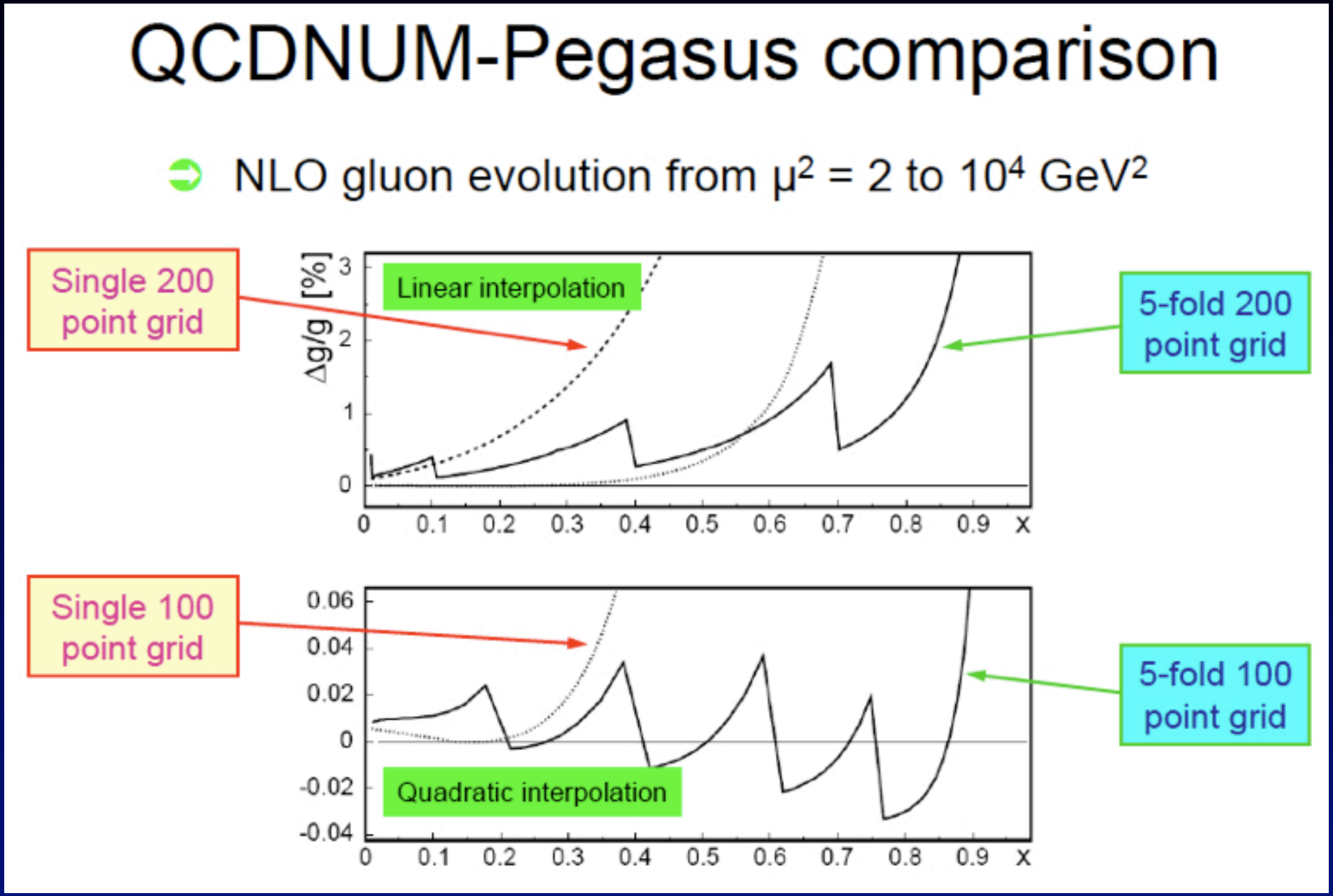
* Set LO, NLO, NNLO
* Input strong coupling constant
* FFNS, VFNS and thresholds $Q^2_{c,b,t}$

QCDNUM: evolution of all PDFs

```
call QCINIT(6,' ')
call GXMAKE(xmin,1,1,nxin,nx,iosp)
call GQMAKE(qq,wt,2,nqin,nq)
call FILLWT(0,id1,id2,nwords)
call SETORD(3)
call SETALF(as0,r20)
call SETCBT(0,iqc,iqb,iqt)
call EVOLFF(func,def,iq0,eps)
call PDFSXQ(x,q,pdf,0)
```

* Function **func** provides input PDFs at Q^2_0
* Array **def** describes flavour composition
* Several routines to return PDFs at x, Q^2

How do we know that QCDNUM is correct?

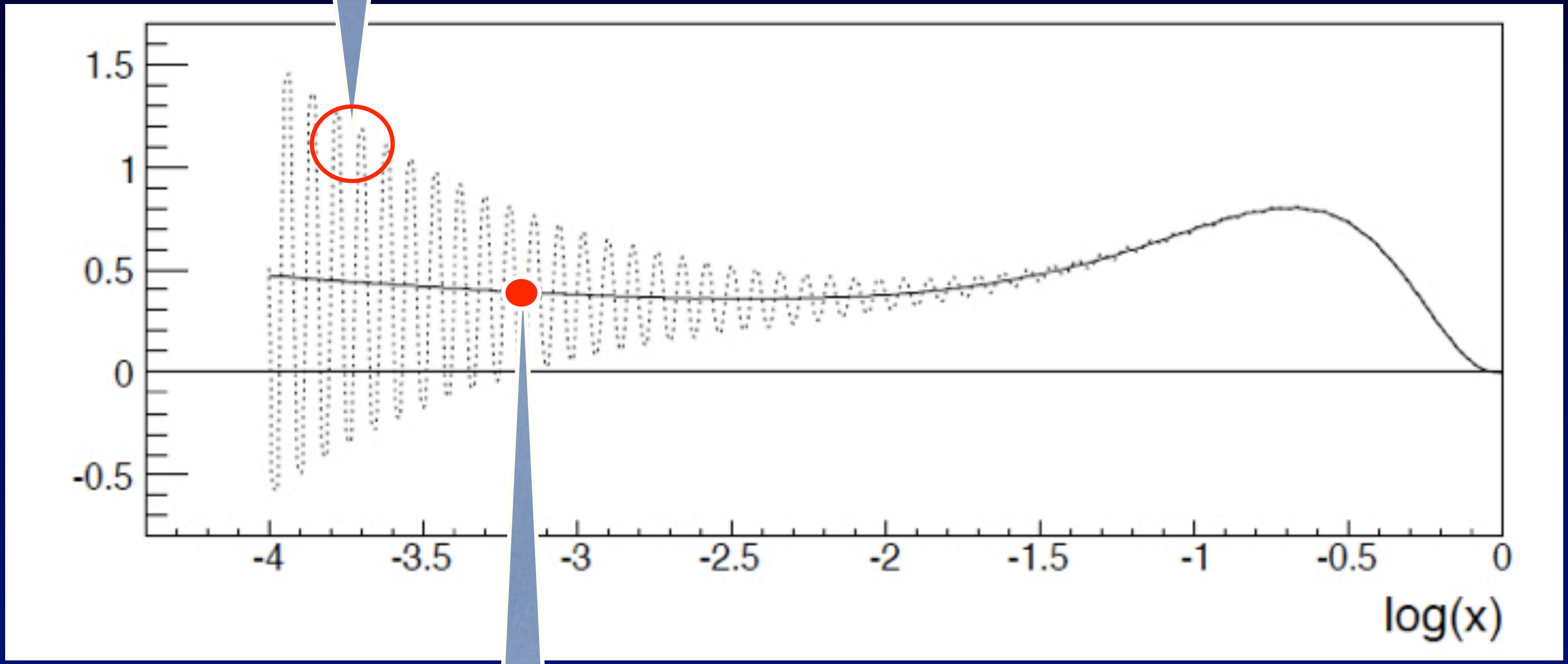


☑ Comparison QCDNUM - PEGASUS $O(10^{-4})$

A. Vogt, CPC 170 (2005) 65

QCDNUM caveat: backward evolution

Backward evolution with quadratic splines may oscillate (forward evolution never oscillates neither do linear splines)



QCDNUM can handle this instability but quad backward evolution over a large range in Q^2 is not recommended

Convolution Engine

$$f \otimes C \equiv x \int_{\chi}^{1} \frac{\mathrm{d}z}{z} f(z, \mu^2)\, C\left(\frac{\chi}{z}, \mu^2, Q^2, m_{\mathrm{h}}^2\right)$$

R.S. Thorne and W.K. Tung, arXiv:0903.3861 (2009)

- Uses rescaling variable, like: $\chi \equiv a x = \left(1 + \frac{m_{\mathrm{h}}^2}{Q^2}\right) x$
- C(...) and a(...) must be supplied as Fortran functions
- You can generate weight tables at initialization and then enjoy very fast convolution as weighted sum

- QCDNUM can handle singularities

$$C = A + [B]_+ + R[S]_+ + D\delta(1-x)$$

- Each term has its own Makewt routine

Store — Coefficient function

```
call MAKEWTA(w,id,afun,achi)
call MAKEWTB(w,id,bfun,achi,0)
call MAKEWRS(w,id,rfun,sfun,achi,0)
call MAKEWTD(w,id,dfun,achi)
```

Table identifier — Defines rescaling variable

How to get your Structure Function

- Generate weight tables at initialization
- Write a structure function function, like

```
function stf(ix,iq)
fcc = FCROSSC(w,idw,idf,ix,iq)
stf = GETALFN(iq,n,ierr)*fcc
return
```

- Pass this function to an interpolation routine

```
call STFUNXQ(stf,x,Q2,Fval,1,0)
```

QCDNUM-17-beta-05

- MBUTIL pool of utility routines (incl. write-up)
- QCDNUM evolution program (incl. write-up)
  - ☑ Evolution fully NNLO
  - ☑ Renormalization scale dependence
  - ☑ Convolution engine fully operational
- ZMSTF zero-mass structure function add-on
  - ☑ F_2, F_L, xF_3, F_L' up to NNLO
  - ☑ Factorisation scale dependence
- HQSTF heavy quark stfs in 3-flavour FFNS
  - ☑ F_2, F_L contribution from (c,b,t) up to NLO
  - ☑ Factorisation scale dependence

Fast?

- 100x50 point 5-fold grid $x > 10^{-5}$ and $Q^2 < 10^4$ GeV^2
- 1000 NNLO evolutions of 11 PDFs (no top) in the VFNS
- For each evolution 1000 NNLO $F_2 + F_L$ in HERA kin range
- Code compiled with gfortran (w/o array boundary chk)
- MacBook 2GHz Intel Core 2 Duo

Routine	Calls	CPU sec	CPU/call
Evolution	1000	42	0.042
F_2, F_L	2.10^{6}	80	4.10^{-5}

✓ Takes 2 minutes which is pretty fast!

Are we done?

- With this talk, yes
- With QCDNUM, almost:
  - Timelike evolution (of fragmentation functions)
  - Evolution of polarised PDFs
  - Convolution of PDFs (parton luminosities)

✓ Stay tuned on **www.nikhef.nl/~h24/qcdnum**

```
                 ///                                  .().
                (..)                                  (--)
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 |                                                                     |
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 |        ##                                                           |
 |                                                                     |
 |       Version 17-beta-05  28-07-09   Author m.botje@nikhef.nl       |
 |                                                                     |
 +---------------------------------------------------------------------+

FILLWT: start weight calculations
Subgrids    5 Subgrid points   22   20   18   16   60
Pij LO    for ospline = 2
Pij NLO   for ospline = 2
Pij NNLO  for ospline = 2
Pij LO    for ospline = 3
Pij NLO   for ospline = 3
Pij NNLO  for ospline = 3
Aij NNLO  for ospline = 3
FILLWT: weight calculations completed


ZMFILLW: start weight calculations   4  41   0   0
ZMFILLW: calculations completed
```

http://www.nikhef.nl/~h24/qcdnum