NNLO Upgrade of QCDNUM

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What is QCDNUM

- QCDNUM is a Fortran program that performs numerical DGLAP evolution of parton densities on a discrete grid in x and μ^2
- QCDNUM provides
  - Evolution of α_s
  - Evolution of unpolarized parton densities
  - Calculation of the structure functions F_2, F_L and xF_3
  - Possibility to independently vary the renormalization and factorization scales
- All this up to NNLO in QCDNUM17

QCDNUM has a long history…

1988	Original code by Ouraou and Virchaux (BCDMS)	CRAY vectorized Fortran	~15 min
1993	NMC adaptation to low x	CRAY vectorized Fortran	~15 min
1998	QCDNUM16.12 used by ZEUS	Unix Fortran77	~10 min
2007	NNLO upgrade QCDNUM17	Unix Fortran77	~1-5 min

QCDNUM17 Beta release ~today

What is new in QCDNUM17

- Fully NNLO
- Automatic separation of PDFs into singlet and non-singlet distributions
- Quadratic spline interpolation
- New very fast evolution algorithm on multiple equidistant grids
- Two alternative definitions of F_L

➲ User friendly, fast, accurate

Singlet/gluon evolution

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

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

Non-singlet evolution

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

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

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

	LO	NLO	NNLO
q_{ij}^{+}	P_{qq}	P_{+}	P_{+}
q_{ij}^{-}	P_{qq}	P_{-}	P_{-}
$q_{\rm v}$	P_{qq}	P_{-}	$P_{\rm v}$

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

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

QCDNUM supports two evolution schemes

- FFNS: number of active flavors is kept constant $3 < n_f < 6$ for all μ^2
- VFNS: number of flavors changes from n_f to n_f+1 at the thresholds μ_c^2, μ_b^2 and μ_t^2
  - At LO and NLO, α_s and the PDFs are continuous at the thresholds
  - At NNLO there are discontinuities in α_s and the PDFs

Chetrikrin et al., PRL 79(1997)2184
Buza et al.,EPJ C1(1998)301

Renormalization scale dependence

- QCDNUM supports a linear relation between the renormalization and factorization scale

$$\mu_{\rm R}^2 = a_{\rm R}\,\mu_{\rm F}^2 + b_{\rm R}$$

- Affects α_s used in the perturbative expansions

$$P_{ij}(x,\mu^2) = a_{\rm s}(\mu^2)\;P_{ij}^{(0)}(x) + a_{\rm s}^2(\mu^2)\;P_{ij}^{(1)}(x) + a_{\rm s}^3(\mu^2)\;P_{ij}^{(2)}(x)$$

- ➲ Renormalization scale dependence affects both the PDFs and the structure functions

Factorization scale dependence

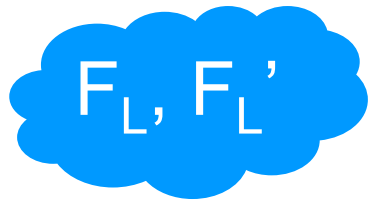
- Likewise $Q^2 = a_{\rm Q}\,\mu_{\rm F}^2 + b_{\rm Q}$
- Affects only F_2, $F_{\rm L}$, xF_3 but in a complicated way...

$$\mathbf{C}_i^{(0)} \to \mathbf{C}_i^{(0)} \qquad \mathbf{C}_i^{(k)} \to \mathbf{C}_i^{(k)} + \sum_{m=1}^{k} \mathbf{C}_i^{(k,m)} L_{\rm F}^m$$

$$\begin{aligned}
\mathbf{C}_i^{(1,1)} &= \mathbf{C}_i^{(0)} \otimes \mathbf{P}^{(0)} \\
\mathbf{C}_i^{(2,1)} &= \mathbf{C}_i^{(0)} \otimes \mathbf{P}^{(1)} + \mathbf{C}_i^{(1)} \otimes \left[\mathbf{P}^{(0)} - \beta_0\,\mathbf{I}\right] \\
\mathbf{C}_i^{(2,2)} &= \frac{1}{2}\,\mathbf{C}_i^{(1,1)} \otimes \left[\mathbf{P}^{(0)} - \beta_0\,\mathbf{I}\right] \\
\mathbf{C}_i^{(3,1)} &= \mathbf{C}_i^{(0)} \otimes \mathbf{P}^{(2)} + \mathbf{C}_i^{(1)} \otimes \left[\mathbf{P}^{(1)} - \beta_1\,\mathbf{I}\right] + \mathbf{C}_i^{(2)} \otimes \left[\mathbf{P}^{(0)} - 2\beta_0\,\mathbf{I}\right] \\
\mathbf{C}_i^{(3,2)} &= \frac{1}{2}\left\{\mathbf{C}_i^{(1,1)} \otimes \left[\mathbf{P}^{(1)} - \beta_1\,\mathbf{I}\right] + \mathbf{C}_i^{(2,1)} \otimes \left[\mathbf{P}^{(0)} - 2\beta_0\,\mathbf{I}\right]\right\} \\
\mathbf{C}_i^{(3,3)} &= \frac{1}{3}\mathbf{C}_i^{(2,2)} \otimes \left[\mathbf{P}^{(0)} - 2\beta_0\,\mathbf{I}\right].
\end{aligned}$$

- F_L is calculated as the convolution of a parton density and a coefficient function

$$F_{\mathrm{L}} = \sum_{i=g,q,\bar{q}} C_{\mathrm{L},i} \otimes f_i$$



- The usual expansion of C_L gives a vanishing F_L at LO

$$C_{\mathrm{L},i} = 0 + a_{\mathrm{s}}\, C^{(1)}_{\mathrm{L},i} + a^2_{\mathrm{s}}\, C^{(2)}_{\mathrm{L},i}$$

➲ QCDNUM supports an alternative F'_L by including a 3-loop coefficient function in the expansion of C_L

$$C_{\mathrm{L},i} = a_{\mathrm{s}}\, C^{(1)}_{\mathrm{L},i} + a^2_{\mathrm{s}}\, C^{(2)}_{\mathrm{L},i} + a^3_{\mathrm{s}}\, C^{(3)}_{\mathrm{L},i}$$

S. Moch et al., PL B606 (2005) 123

Numerical method in a nutshell

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

➲ QCDNUM17 is very fast

A full NNLO analysis in ten lines

```
call QCINIT(6,' ')
call SETORD(iord)
call SETALF(as0,r20)
call SETTHR(nfin,q2c,q2b,q2t)
call GXMAKE(xmin,1,1,nxin,nx,iosp)
call GQMAKE(qq,wt,2,nqin,nq)
call FILLWT(0,id1,id2,nw)
call EVOLFF(func,def,iq0,eps)
call ALLPDF(x,q,pdf,0)
call STRFUN(2,proton,x,q,F2p,1,0)
```

QCDNUM initialization

```
call QCINIT(6,' ')
call SETORD(iord)
call SETALF(as0,r20)
call SETTHR(nfin,q2c,q2b,q2t)
call GXMAKE(xmin,1,1,nxin,nx,iosp)
call GQMAKE(q
call FILLWT(0
call EVOLFF(f
call ALLPDF(x
call STRFUN(2
```

- Initialize QCDNUM
- Set LO, NLO, NNLO
- Set starting value of α_s
- Set FFNS or VFNS
- Set thresholds in the VFNS

Grids and weights

- Define (multiple) *x* grid(s)
- Define spline interpolation order
- Define μ^2 grid

```
call GXMAKE(xmin,1,1,nxin,nx,iosp)
call GQMAKE(qq,wt,2,nqin,nq)
call FILLWT(0,id1,id2,nw)
```

- Partition the internal store
- Calculate weight tables

NNLO evolution of all PDFs

- User supplied function **`func(i,x)`** provides $f_i(x)$ at the input scale μ^2 for the gluon and $2n_f$ quark densities
- The input scale is given by the grid point **`iq0`**
- In the VFNS, **`iq0`** < charm threshold

```
call EVOLFF(func,def,iq0,eps)
```

- The flavor decomposition of each input quark density is given in **`def(-6:6,12)`**

Harvest the results….

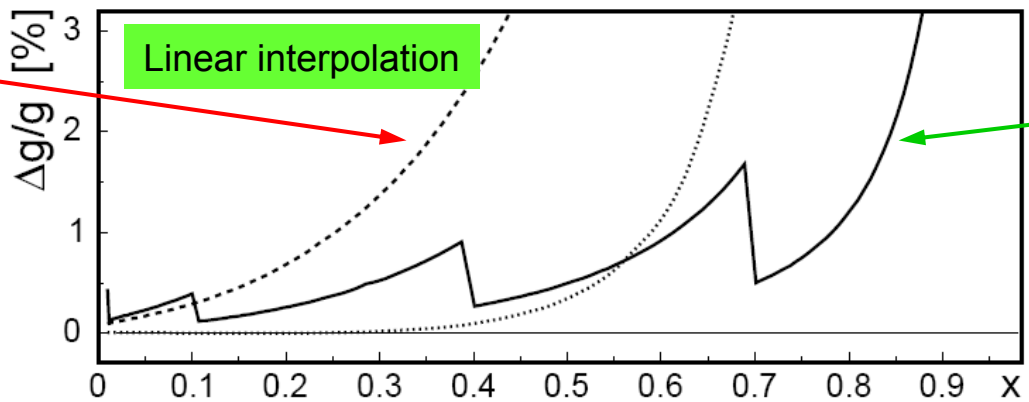
- Interpolate to x and μ^2 and return the densities g, d, u, …, t in **`pdf(-6:6)`**
- Calculate F_2, F_L, F'_L or xF_3 for a linear combination of quarks and anti-quarks as specified in the input **`array(-6:6)`**

```
call ALLPDF(x,q,pdf,0)
call STRFUN(2,proton,x,q,F2p,1,0)
```

QCDNUM-Pegasus comparison

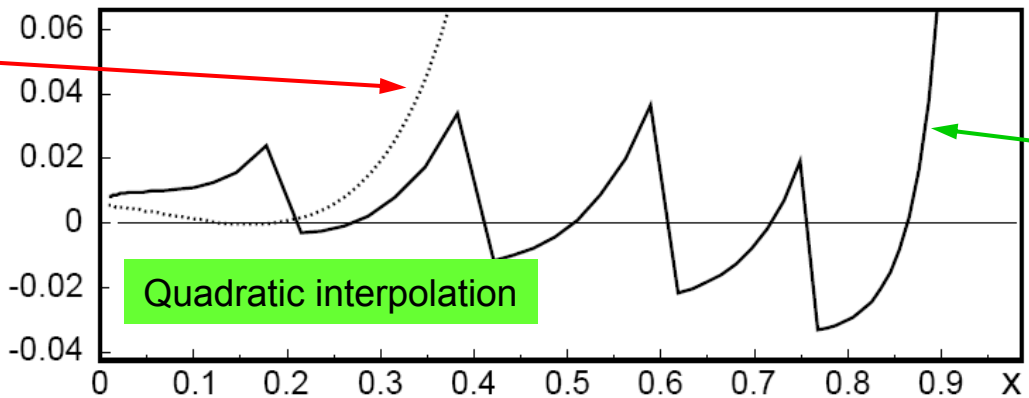
- NLO gluon evolution from $\mu^2 = 2$ to 10^4 GeV^2

Single 200 point grid



5-fold 200 point grid

Single 100 point grid



5-fold 100 point grid

QCDNUM17 accuracy

- NLO gluon evolution from $\mu^2 = 2$ to 10^4 GeV^2 on an x grid down to $x = 10^{-5}$
- Single 200 point grid with linear interpolation
  $\Delta g/g < 2\%$ for $x < 0.35$
- Single 100 point grid with quadratic interpolation
  $\Delta g/g < 2\%$ for $x < 0.65$
- Five-fold 200 point grid with linear interpolation
  $\Delta g/g < 2\%$ for $x < 0.85$
- Five-fold 100 point grid with quad interpolation
  $\Delta g/g < 5 \times 10^{-4}$ for $x < 0.9$
- ☺ Gain in speed by factor of 4 with quadratic interpolation because the number of grid points can be reduced from 200 to 100….

Status of present Beta release

- ☺ PDF and α_s evolution should be OK
- 😐 Renormalization scale dependence implemented but needs some more tests
- 😐 Structure functions implemented but need some more tests
- ☹ Factorization scale dependence not yet implemented
- ☹ Alternative F'_L not yet available

To Summarize…

- QCDNUM17 is basically OK but might still need a bit of shakedown
- Factorization scale dependence and alternative F_L will soon be implemented
- You can get the current Beta release and write-up from

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