QCDNUM Status and Plans

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QCDNUM releases

- 17-01/14: Released 21-Dec-2017
  - C++ interface for out-of-the-box, ZMSTF and HQSTF

arXiv:1712.08162

- 17-01/15: Will be released today ☺
  - Out-of-the-box evolution routine with intrinsic heavy flavours
  - New out-of-the-box singlet/non-singlet evolution routine
  - New routine to set cuts in the kinematic plane
  - More flexibility in setting thresholds
  - Evolution start scale can be anywhere in μ^2
  - Pdf access not anymore restricted to those with current parameters

Backward compatible (almost)
Just install 17-01/15 and enjoy the added features

Scheme selection and threshold settings

```
call SETCBT( nfix, iqc, iqb, iqt )
```

Scheme	nfix	Thresholds	
FFNS	3/4/5/6	No flavour thresholds	
VFNS	0	iqc	Boundary nf = 3/4
		iqb	Boundary nf = 4/5 must be iqb ≥ iqc+2
		iqt	Boundary nf = 5/6 must be iqt ≥ iqb+2

Settings in SETCBT more flexible than before

- EVOLFG has no start point restriction so that one may put any single threshold, or any two consecutive thresholds, or all three thresholds

NEW

- nfix = 0 : select VFNS with dynamic heavy flavours
- nfix = 1 : select VFNS with intrinsic heavy flavours (see later)

NEW

Reminder: two μ^2 grids

- Internally a threshold is stored twice
  - With n_f above threshold
  - With n_f below threshold
- The user sees two grids
  - `iq = +iqh` : n_f above threshold (456-grid)
  - `iq = -iqh` : n_f below threshold (345-grid)
- To see charm matching discontinuity, for instance:

```
FVALIJ(iset,id,ix,+iqc,1) – FVALIJ(iset,id,ix,-iqc,1)
```

Updated EVOLFG routine

```
call EVOLFG(itype,func,def,iq0,epsi)
```

`itype`	Select polarised/unpolarised/time-like
`func(j,x)`	Input pdfs $f_j(x)$ at the input scale `iq0`
`def(i,j)`	Contribution of (anti)quark flavour `i` to input pdf `j`
`iq0`	Starting scale of the evolution
`epsi`	Output smoothness indicator to detect oscillations

Same argument list as before but more flexible NEW

- `itype` now allows you to select the output pdf set
- `iq0` can be anywhere within the grid or cuts
- `func` accepts parameterisation of intrinsic heavy flavours

Output pdf set selection in EVOLFG

- Evolution type selection via itype allows for direct storage of evolved pdfs into any pdf set [1-24]

1	Evolve unpolarised pdfs in iset=1	
2	Evolve polarised pdfs in iset=2	
3	Evolve fragmentation fcs in iset=3	
10*iset+itype	Evolve 1, 2 or 3 and store in iset	NEW

- Thus itype=52 stores polarised pdfs in set 5, etc.
- This provides an alternative to copying pdf set 1, 2, 3 to another set with PDFCPY

Start scale in EVOLFG

- Previously the VFNS start scale had to be below the charm threshold: evolution always started at nf = 3
- Now the VFNS start scale can be anywhere inside the grid: evolution can start at nf = 3, 4, 5, 6 NEW
- When you start the evolution at a threshold `iqh`:

```
iq0 = +iqh : Start with nf above the threshold
             Do the matching in backward evolution
iq0 = -iqh : Start with nf below the threshold
             Do the matching in forward evolution
```

Reminder

QCDNUM back evolution is iterative but reasonably accurate

To see what EVOLFG does exactly

```
call SETINT('edbg',1)
```

NEW

```
------------------ forward ------------------
EVOLVE iq1,2 =     9    9   nf =    3  start
JUMPNF iq1,2 =     9    9   nf =    3  4
EVOLVE iq1,2 =     9   18   nf =    4
JUMPNF iq1,2 =    18   18   nf =    4  5
EVOLVE iq1,2 =    18   44   nf =    5
JUMPNF iq1,2 =    44   44   nf =    5  6
EVOLVE iq1,2 =    44   60   nf =    6
------------------ reverse ------------------
EVOLVE iq1,2 =     9    1   nf =    3  start
```

iq0 = -iqc

3 -> 4 transition forward evolution

```
------------------ forward ------------------
EVOLVE iq1,2 =     9   18   nf =    4  start
JUMPNF iq1,2 =    18   18   nf =    4  5
EVOLVE iq1,2 =    18   44   nf =    5
JUMPNF iq1,2 =    44   44   nf =    5  6
EVOLVE iq1,2 =    44   60   nf =    6
------------------ reverse ------------------
EVOLVE iq1,2 =     9    9   nf =    4  start
JUMPNF iq1,2 =     9    9   nf =    4  3
EVOLVE iq1,2 =     9    1   nf =    3
```

Here is an example showing what happens when we start the evolution at the charm threshold with 3 (-iqc) or 4 (+iqc) flavours

iq0 = +iqc

4 -> 3 transition reverse evolution

New EVSGNS routine

```
call EVSGNS(itype,func,isns,n,iq0,epsi)
```

NEW

`isns(i)`	Type of evolution (singlet/gluon, non-singlet)
`n`	Number of evolutions

Creates a user-pdf set with n+1 pdfs

- It is not possible to match arbitrary sets of pdfs so that the evolution can only run in the FFNS or MFNS
- There is also a routine to import arbitrary pdf sets

```
call USRPDF(func,iset,n,offset,epsi)
```

NEW

Input pdfs for n_f active flavours

- Input pfs are parameterised in `func(j,x)`

```
function func(j,x)

if(j.eq.-1) initialise func

if(j.eq. 0) func = gluon(x)
if(j.eq. 1) func = pdf01(x)
 ..
if(j.eq.12) func = pdf12(x)

return
end
```

Dummy call with `j = -1`

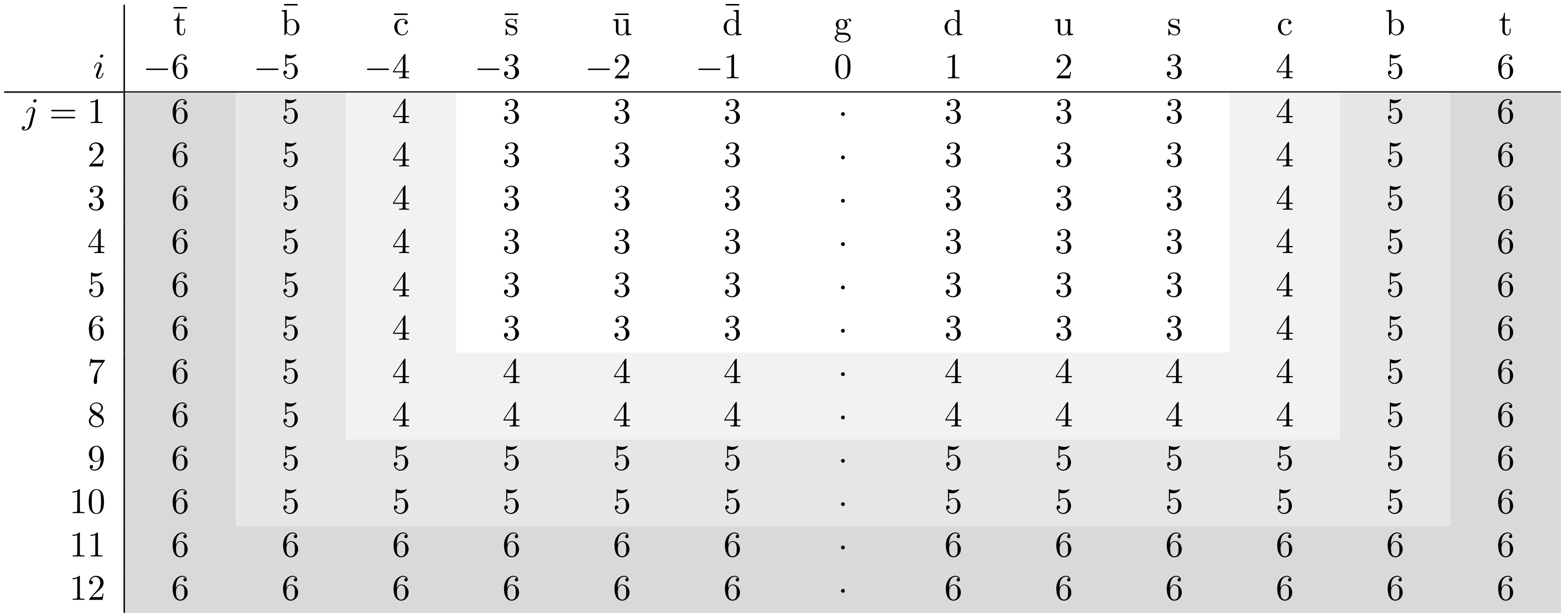
NEW

- Called for the `j` = `0`, …, `2nf` input pdfs at μ_0^2

- Parameterisations for `j` > `2nf` are ignored

Flavour composition of input pdfs

- Contribution of flavour `i` to $\mathtt{f}_\mathtt{j}$ is given in `def(i,j)`



	$\bar{t}$	$\bar{b}$	$\bar{c}$	$\bar{s}$	$\bar{u}$	$\bar{d}$	g	d	u	s	c	b	t
i	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6
$j = 1$	6	5	4	3	3	3	·	3	3	3	4	5	6
2	6	5	4	3	3	3	·	3	3	3	4	5	6
3	6	5	4	3	3	3	·	3	3	3	4	5	6
4	6	5	4	3	3	3	·	3	3	3	4	5	6
5	6	5	4	3	3	3	·	3	3	3	4	5	6
6	6	5	4	3	3	3	·	3	3	3	4	5	6
7	6	5	4	4	4	4	·	4	4	4	4	5	6
8	6	5	4	4	4	4	·	4	4	4	4	5	6
9	6	5	5	5	5	5	·	5	5	5	5	5	6
10	6	5	5	5	5	5	·	5	5	5	5	5	6
11	6	6	6	6	6	6	·	6	6	6	6	6	6
12	6	6	6	6	6	6	·	6	6	6	6	6	6

- EVOLFG takes $\mathtt{2n}_\mathtt{f}$ × $\mathtt{2n}_\mathtt{f}$ sub-matrix and ignores the rest

- Independent pdf input requires non-singular sub-matrix

VFNS with intrinsic heavy flavours

- Set `nfix` = 1 in upstream call to SETCBT NEW
- Provide parameterisation in `func(j,x)` for `j` > $2n_f$
- Specify flavour composition in `def(i,j)` for `j` > $2n_f$
  - Accepts only a linear combination of h and hbar without admixture of other flavours
  - Row of zero's terminates the heavy flavour input
- Input provides scale-independent density below threshold and evolution start point at threshold

NB: input heavy flavours at μ_0^2 are <u>always</u> intrinsic

Matching with intrinsic heavy flavours

R.D. Ball et al.
PLB754, 49 (2016)
arXiv:1510.00009

- More complicated since heavy quark enters the game at NLO

$$
\begin{aligned}
\Delta g &= a_{\mathrm{s}}\, A_{\mathrm{gh}} \otimes h^{+} + a_{\mathrm{s}}^{2}\, \{A_{\mathrm{gq}} \otimes q_{\mathrm{s}} + A_{\mathrm{gg}} \otimes g\} \\
\Delta h^{+} &= a_{\mathrm{s}}\, A_{\mathrm{hh}} \otimes h^{+} + a_{\mathrm{s}}^{2}\, \{A_{\mathrm{hq}} \otimes q_{\mathrm{s}} + A_{\mathrm{hg}} \otimes g\} \\
\Delta h^{-} &= a_{\mathrm{s}}\, A_{\mathrm{hh}} \otimes h^{-} \\
\Delta q_i^{\pm} &= a_{\mathrm{s}}^{2}\, A_{\mathrm{qq}} \otimes q_i^{\pm}
\end{aligned}
$$

BMSN (NNLO)

- Difficulty: the QCDNUM pdf basis maximally decouples DGLAP but not the matching equations
- Therefore transform to a basis that better decouples the ME
- Reverse matching is numerically unstable ⇒ iterative solution
- All this is documented in the write-up Appendix C and D

Cuts in the kinematic plane

```
call SETLIM(ixmin,iqmin,iqmax,dum)
```

NEW

- Set kinematic cuts for
  - Next evolution by EVOLFG or EVDGLAP (toolbox)
  - Next pdf import by EXTPDF
- To release cut set parameter to zero
- Useful for speeding-up pdf fits
  - In χ^2 loop limit evolution to kinematic range of the data
  - After convergence evolve, only once, on full grid
- Useful to define kinematic range of imported pdf set

Evolution parameter keys

- There are 12 parameters divided in 6 groups

1. order (1)
2. α_s (2-3)
3. thresholds (4-7)
4. scale (8-9)
5. cuts (10-12)
6. all (1-12)

- All settings are stored in a repository and given a version number (key): (un)equal keys means (un)equal parameters
- Handy for quick checks on parameter groups NEW
- E.g. pdf sets with the same threshold settings have

```
KEYGRP(iset1,3) == KEYGRP(iset2,3)
```

Summary of new subroutines

`WTFILE`	Maintain an up-to-date weight file on disk
`NFRMIQ`	Number of flavours vs μ^2 for a given pdf set
`SETLIM`	Set evolution limits
`GETLIM`	Get current limits
`KEYGRP`	Key (version number) of a parameter group
`EVSGNS`	Evolve an arbitrary set of singlet/non-singlet pdfs
`USRPDF`	Import an arbitrary pdf set
`IEVTYP`	Get evolution type of a pdf set
`FFPLOT`	Generate plot file (for gnuplot)

Pdf access

- PDF tables are somewhat complicated objects with a μ^2 subgrid structure, depending on the threshold settings

- Subgrids are handled by fast pointer-tables

- There used to be one pointer-table for the current settings which restricted pdf access to those settings only

- Now every pdf set has its own pointer-table so that access is not anymore restricted

Change of basis

- There are two changes in the basis definition
  - $e_2 = u - d$ has changed to $d - u$
  - $e_h = h^{\pm}$ for heavy quarks below threshold
- This should not affect your code unless you use the basis pdfs instead of the flavour pdfs
- The reason for these changes is the introduction of a fast transformation algorithm, including transformation to a special basis for intrinsic heavy quark matching

Performance

- Standard timing test of 1000 evolutions and 2M structure function calculations (mimic a pdf fit)
- On a MacBook Pro 2018 this gives

5.7 sec	QCDNUM-17-01/14
6.2 sec	QCDNUM-17-01/15

- About 10% speed penalty for 17-01/15
- Modest price for a lot of increased flexibility

Accuracy of iterative reverse evolution

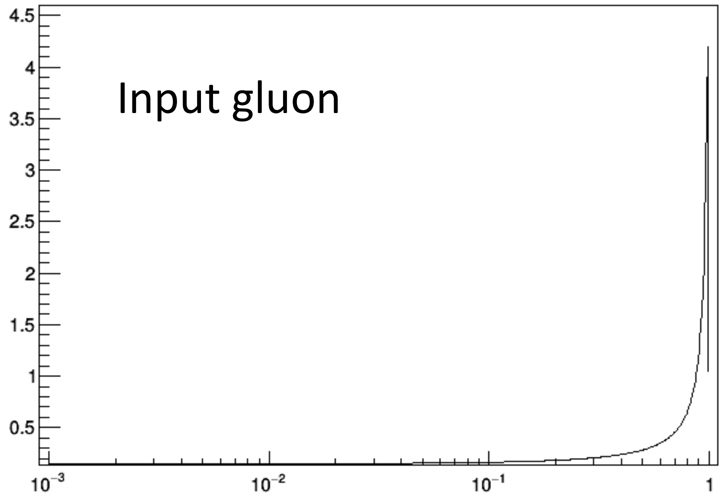
- Do NNLO VFNS evolution
- Evolve from 2 to 10^4 GeV^2 and then back to 2 GeV^2
- Compare forward and reverse evolution for all 13 basis pdfs

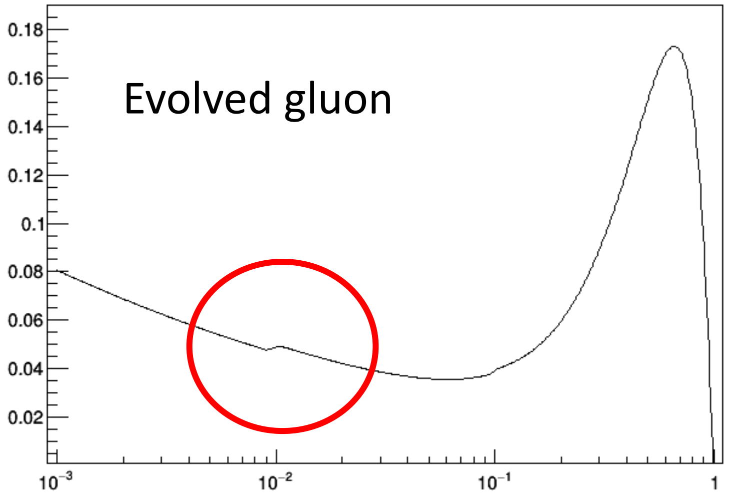
```
id =  0      dif =  0.0014
id =  1      dif =  0.0019
id =  2      dif =  0.0018
id =  3      dif =  0.0019
id =  4      dif =  0.0016
id =  5      dif =  0.0001
id =  6      dif =  0.0000
id =  7      dif =  0.0019
id =  8      dif =  0.0018
id =  9      dif =  0.0019
id = 10      dif =  0.0000
id = 11      dif =  0.0000
id = 12      dif =  0.0000
```

Small hiccup

- Pomeron evolution with input gluon peaked at very large x
- Multiple x-grids show up in the evolved gluon (and singlet)
- Will be improved in the next QCDNUM release

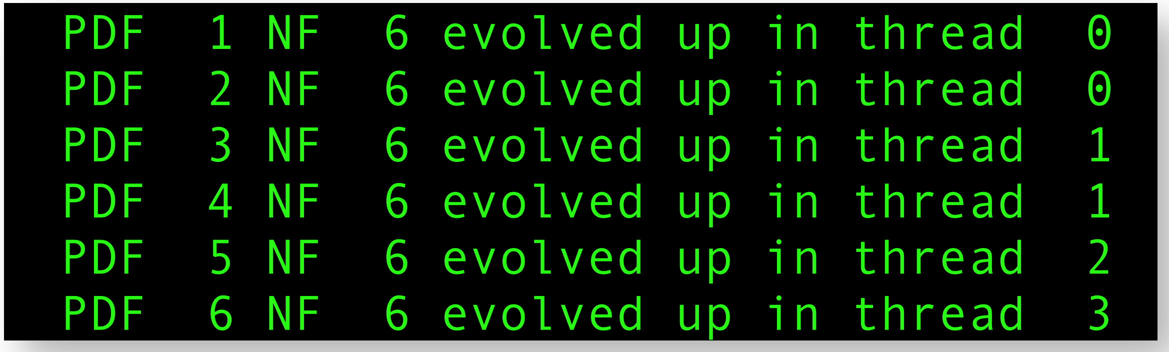
Thanks to Daniel Britzger for spotting the problem





EVOLSG threading with OpenMP

- At fixed nf, the 2nf singlet and nonsinglet evolutions can in principle be run in parallel (up to 12 evolutions)
- OpenMP directives are not yet implemented but by design the new EVOLSG routine should be thread-safe
- Proof of principle in MickeyMouse code: fake evolution of 6 pdfs distributed over 4 threads on my MacBook



```
 PDF   1 NF   6 evolved up in thread  0
 PDF   2 NF   6 evolved up in thread  0
 PDF   3 NF   6 evolved up in thread  1
 PDF   4 NF   6 evolved up in thread  1
 PDF   5 NF   6 evolved up in thread  2
 PDF   6 NF   6 evolved up in thread  3
```

- Might become quite a CPU saver when it all works …

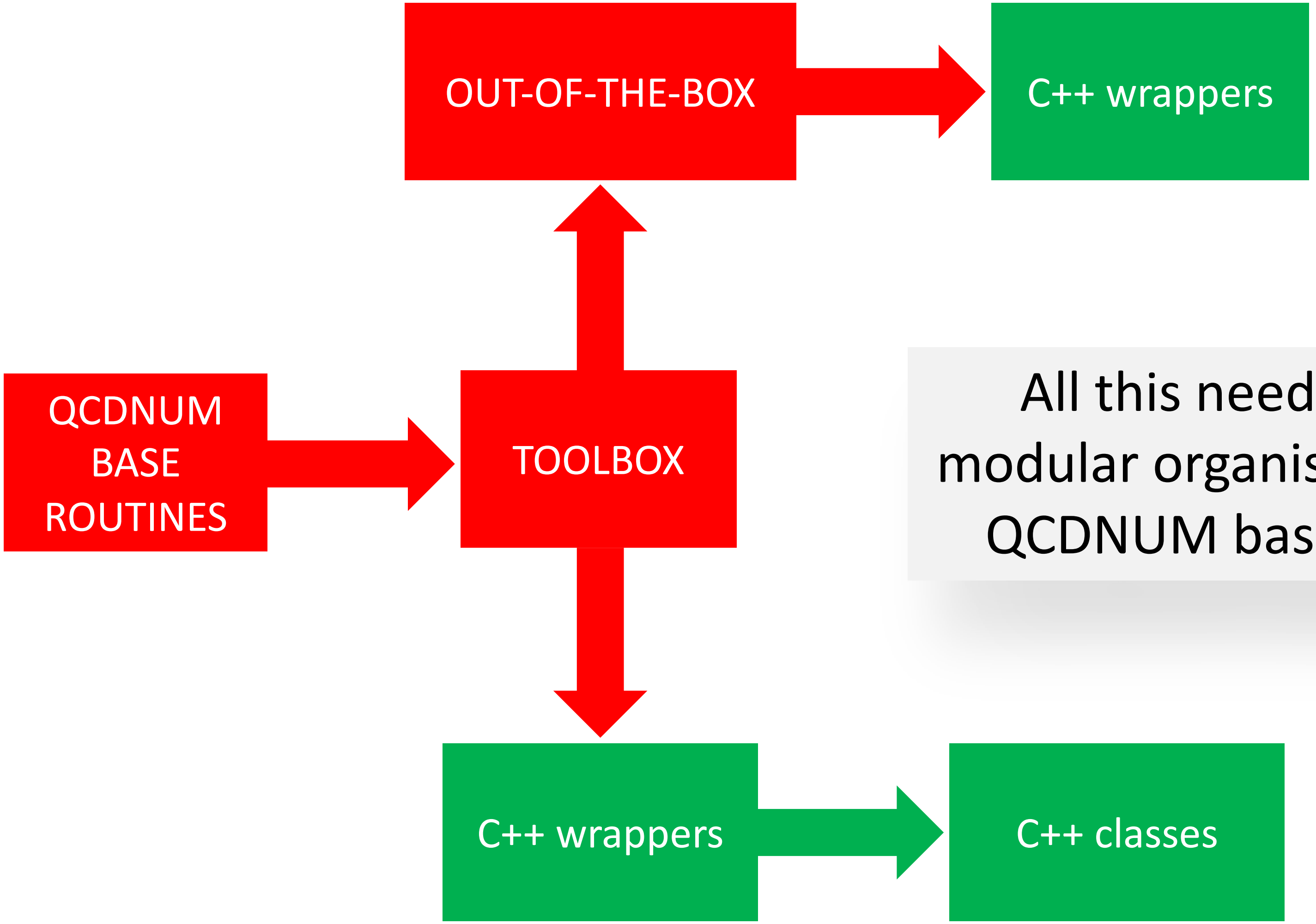
QCDNUM short-term todo list

- Put OpenMP directives in EVOLSG for parallel running
- Better handling of multiple x-grids
- Upgrade polarised and time-like evolution to NNLO
- Turn Renats QCD-QED code into a QEDEVOL package (this is after a re-design of the toolbox)

Long-term code development

- QCDNUM memory is a collection of table sets stored in a large linear array (workspace)
- Routines that operate on a set only care about the position (base address) of table sets in the workspace
- Thus we can have one large workspace with many sets (FORTRAN) or many workspaces with one set (C++)
- In this way table sets can become objects of a C++ class and C++ wrappers of FORTRAN routines can become member functions of that class

Long-term program structure



All this needs a more modular organisation of the QCDNUM base routines

- There are a lot of internal changes in 17-01/15
- Code passes all my tests
- But please stress-test the program in xFitter and report problems to me