QCDNUM Status and Plans

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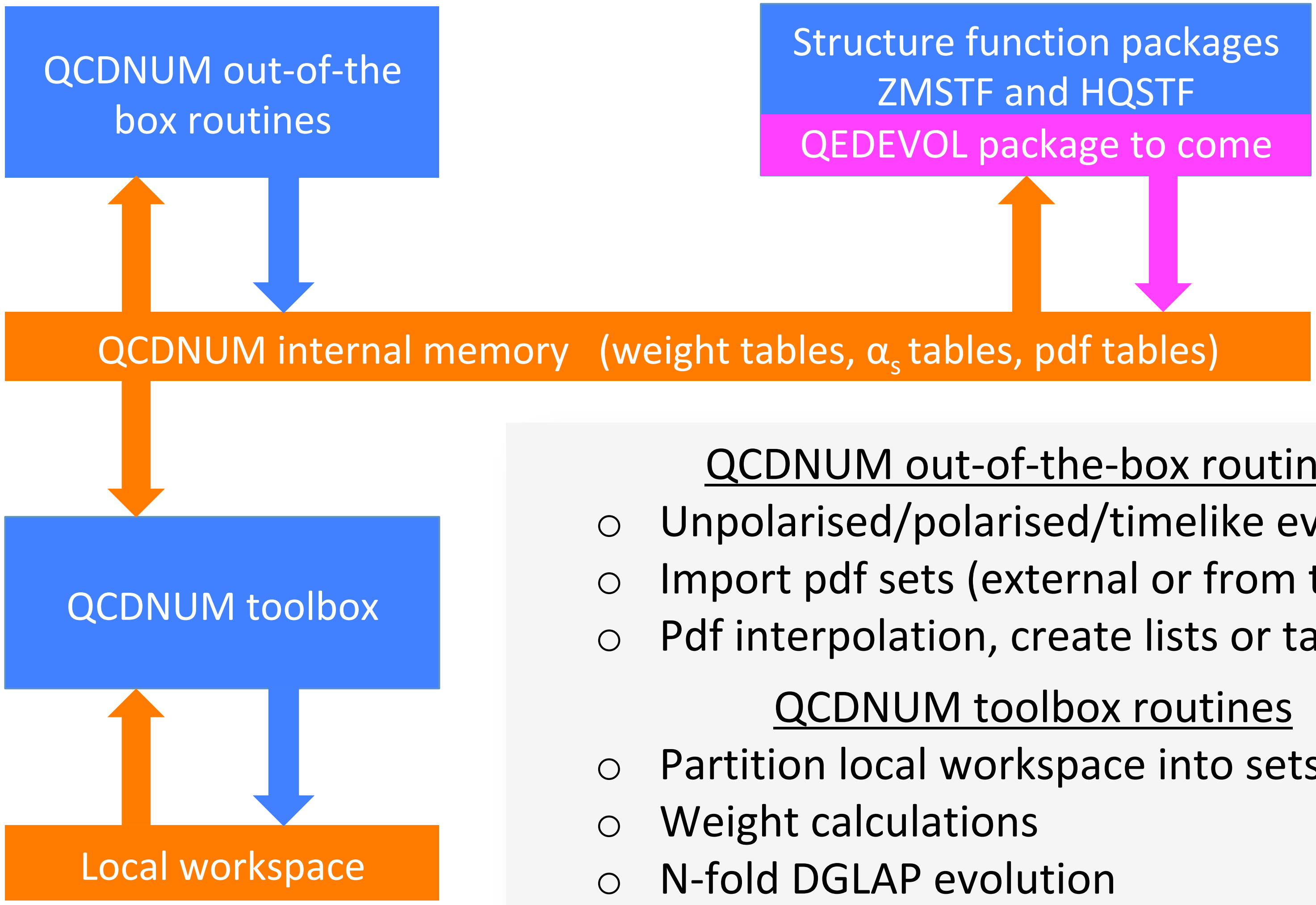
xFitter external workshop

Krakow March 6, 2018

QCDNUM program structure


QCDNUM out-of-the box routines
Structure function packages ZMSTF and HQSTF
QEDEVOL package to come
QCDNUM internal memory (weight tables, α_s tables, pdf tables)
QCDNUM toolbox
Local workspace

QCDNUM out-of-the-box routines

- Unpolarised/polarised/timelike evolution
- Import pdf sets (external or from toolbox)
- Pdf interpolation, create lists or tables

QCDNUM toolbox routines

- Partition local workspace into sets of tables
- Weight calculations
- N-fold DGLAP evolution
- Convolution tools, fast convolution engine

QCDNUM releases

Website
http://www.nikhef.nl/user/h24/qcdnum

- 17-00/08: Stable release
  - Bug fix in singlet time-like evolution (Feb 2016)

arXiv:1602.08383

- 17-01/XX: Pre-releases on the road to QCDNUM-18-00
  - Suite of toolbox routines for N-fold DGLAP evolution
  - Imported pdf sets can have pdfs beyond qluon and quarks
  - Can store pdf sets with different evolution parameters
  - New very fast pdf interpolation routines
- 17-01/14: Released 21-Dec-2017
  - C++ interface for out-of-the-box, ZMSTF and HQSTF

arXiv:1712.08162

- 17-01/15: Almost ready
  - New out-of-the-box evolution routine with intrinsic heavy flavours
  - New routine to set cuts in the kinematic plane

C++ or FORTRAN77, thats the question

- QCDNUM is fast mainly because of
  - Code written in FORTRAN77
  - Very fast addressing by an in-house memory manager
- Recoding in C++ would be a huge effort and most likely will lead to quite some speed penalties
- Decide not to recode but to provide C++ interface
- Interface initially written by Valerio Bertone (thanks!)
- Fully operational in 17-01/14 except for the toolbox

C++ interface to QCDNUM

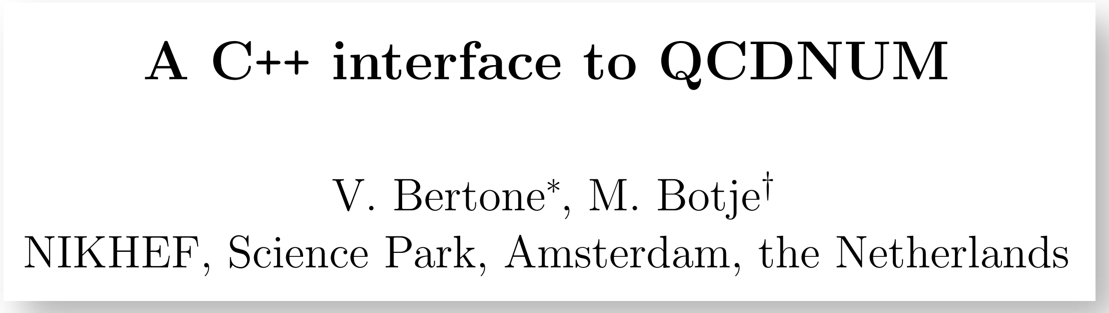
- Very easy to use, basically,

```
call SUB(arguments)
```

⇓

```
QCDNUM::sub(arguments);
```

- Documented in the write-up and in ArXiv:1712.08162



A C++ interface to QCDNUM

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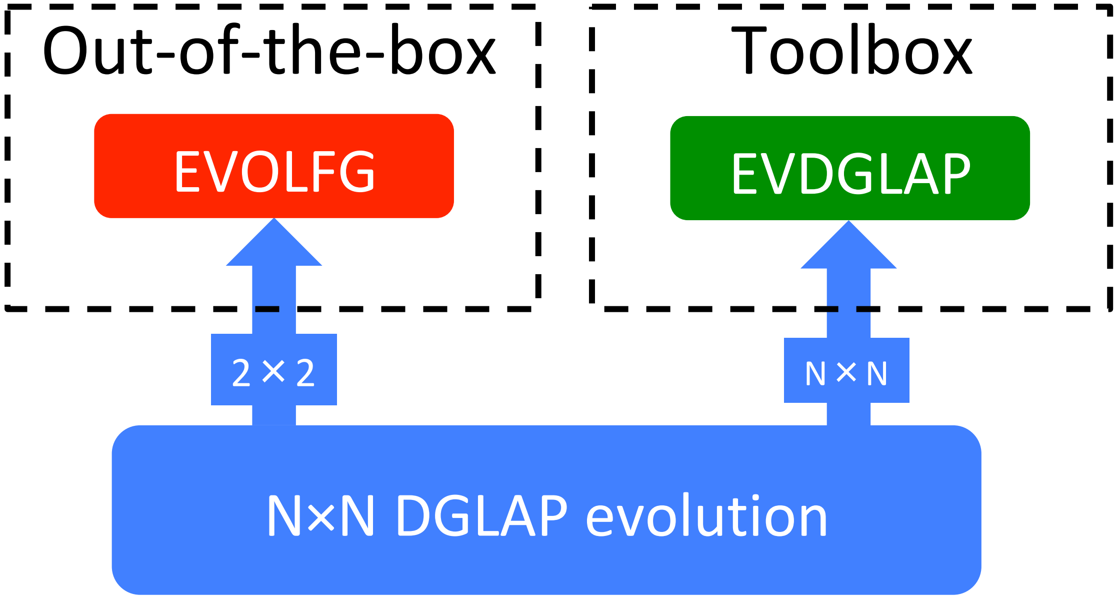
QCDNUM-17-01/15 almost done

- Replaced old 2-fold DGLAP routine by an interface to the toolbox N-fold evolution routine



- Had to speed-up N-fold DGLAP by factor 2
- Present speed penalty only 10-20% ☺

New 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

<u>Reminder</u>

Avoid QCDNUM back evolution as much as possible

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

Input pdfs for n_f active flavours

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

```
function func(j,x)
if(j.eq. 0) func = gluon(x)
if(j.eq. 1) func = pdf01(x)
 ..
if(j.eq.12) func = pdf12(x)
return
end
```

- Called for the `j` = `0`, …, `2n`$_f$ input pdfs at μ_0^2
- Parameterisations for `j` > `2n`$_f$ are ignored

Flavour composition of input pdfs

- Contribution of flavour `i` to $\mathtt{f_j}$ 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 $\mathtt{2n_f} \times \mathtt{2n_f}$ sub-matrix and ignores the rest
- Independent pdf input requires non-singular sub-matrix

NEW

VFNS with intrinsic heavy flavours

- Set `nfix` = 1 in upstream call to SETCBT
- 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
  - You can set all coefficients to zero to turn heavy flavour off
- Input provides scale-independent density below threshold and evolution start point at threshold

NB: dynamic heavy flavours (`nfix` = 0) are zero below threshold

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)

- Code presently OK for forward but not for reverse matching
- Problem: the QCDNUM pdf basis maximally decouples DGLAP but not the matching equations
- Solution: transform to a basis that better decouples the ME
- Documented in write-up Appendix C, code still to be written

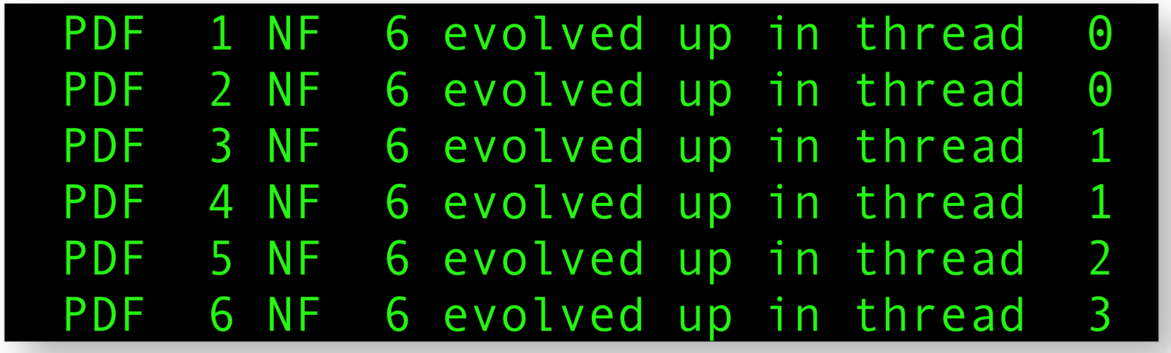
Cuts in the kinematic plane

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

- Set kinematic cuts for
  - Next evolution by EVOLFG or EVDGLAP (toolbox)
  - Next pdf import by EXTPDF
- To release cut set parameter to zero (or outside grid)
- 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

New in EVOLSG: thread-safety

- 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 …

To come: QEDEVOL package

- QCDNUM QCD-QED is already implemented in xFitter and Renat sent me the standalone version of the code
- Turn this into a package with basically two routines:

`QEDWGTS`	To be called instead of `FILLWT`
`QEDEVOL`	To be called instead of `EVOLFG`

- To do in addition:
  – Provide C++ interface
  – Provide thread support
  – Provide small write-up
  – Include the package in the QCDNUM distribution with proper reference to Renat’s work

QCDNUM todo list

- Finalise matching and release QCDNUM-17-01/15
- And then, not in order of priority:
  - Put OpenMP directives in EVOLSG for parallel running
  - Upgrade polarised and time-like evolution to NNLO
  - Turn Renats code into a QEDEVOL package
  - Toolbox: more flexibility through user-defined functions
  - Investigate numerical stability of backward evolution