Interfacing APFEL to HERAFitter

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Why APFEL in HERAFitter

- APFEL is a library that provides a number of functionalities that are useful for PDF fits:
  - fast DGLAP evolution up to NNLO in QCD in the FFN and VFN schemes.
  - LO QED corrections to the DGLAP evolution ⇒ photon PDF.
  - Module for the computation of DIS NC and CC observables in the FONLL scheme, which was the only one missing in HERAFitter.
  - Pole and MSbar heavy quark masses.
  - Scale variations.
  - Different solutions of the DGLAP equation.
  - Lepton PDFs.
  - …

Why APFEL in HERAFitter

- In order to use APFEL in HERAFitter there are two main steps to be taken:

1. interface the **DGLAP evolution** of APFEL to HERAFitter:

   - access to the QCD and QCD+QED evolution.

2. Interface the **DIS module** of APFEL to HERAFitter:

   - access to the DIS structure functions in the FONLL scheme.

DGLAP Evolution

The Strategy

- Two main possibilities:

1. use the current structure based on the QCDNUM functionalities:

   - advantage: easy to code,
   - drawback: non optimal to exploit APFEL.

2. Restructure the code when using APFEL for the evolution:

   - advantage: optimized use of APFEL, *i.e.* better performance,
   - drawback: more work needed.

DGLAP Evolution

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DGLAP Evolution

The Usage

- The first step to take is to install the trunk of APFEL (we will soon tag a version of APFEL to be used with HERAFitter).

- To enable the use of APFEL, one needs to configure HERAFitter giving the following command:

```
./configure --enable-apfel
```

- this will link APFEL when compiling HERAFitter.

- One additional option for `TheoryType` in the steering card:

```
TheoryType = 'DGLAP_APFEL'  ! 'DGLAP'       -- collinear evolution
                            ! 'DGLAP_APFEL' -- collinear evolution with APFEL
                            ! 'DIPOLE'      -- dipole model
                            ! 'uPDF'        -- un-integrated PDFs
                               !uPDF1 fit with kernel ccfm-grid.dat file
                               !uPDF2 fit evolved uPDF, fit just normalisation
                               !uPDF3 fit using precalculated grid of sigma_hat
```

DGLAP Evolution

The Implementation

- When the steering card is read (`read_steer.f`):

```
      if (TheoryType.eq.'DGLAP') then
         iTheory =  0
      elseif (TheoryType.eq.'DGLAP_APFEL') then
         iTheory = 10
         IPDFSET = 7
```

Needed to distinguish the APFEL evolution from QCDNUM

To treat APFEL on the same footing as LHAPDF

- When the evolution is initialized (`init_theory.f`):

```
      if(itheory.eq.0.or.itheory.eq.10) then
C Init evolution code:
         call qcdnum_ini
C Init APFEL if needed
         if(itheory.eq.10) call apfel_ini
```

Initialize the (x,Q) grid in QCDNUM

Initialize APFEL according to the input parameters

DGLAP Evolution

The Implementation

- The initialization of APFEL takes place inside the `apfel.f` file:

```
      call SetTheory("QCD")                  ! Set QCD evolution (default)
      call SetFastEvolution(.true.)          ! Use fast evolution (default)
      call SetAlphaEvolution("exact")        ! Use exact solution on the beta functions (default)
      call SetPDFEvolution("exactalpha")     ! Use DGLAP evolution in terms of alphas (rather than muF => faster for short steps)
      call SetQLimits(0.5d0,20000d0)         ! Evolution limits
      call SetNumberOfGrids(3)               ! x-space grid settings
      call SetGridParameters(1,40,3,9.8d-7)
      call SetGridParameters(2,30,3,1d-2)
      call SetGridParameters(3,20,3,7d-1)
      call LockGrids(.true.)                   ! Lock subgrids
      call SetPerturbativeOrder(I_FIT_ORDER-1)   ! Set perturbative order
      if(HF_SCHEME(1:2).eq."FF")then             ! Set mass scheme for the PDF evolution
         call SetFFNS(3)
      else
         call SetVFNS
      endif
      if(HF_SCHEME(9:12).eq.”RUNM")then
         call SetMSbarMasses(dble(HF_MASS(1)),dble(HF_MASS(2)), ! Heavy-quark thresholds in the MSbar scheme
     1                       dble(HF_MASS(3)))
         call EnableMassRunning(.false.)
         if(HF_SCHEME(14:15).eq."ON") call EnableMassRunning(.true.)
      else
         call SetPoleMasses(dble(HF_MASS(1)),dble(HF_MASS(2)),  ! Heavy-quark thresholds in the Pole scheme
     1                      dble(HF_MASS(3)))
      endif
*
*     Initialize APFEL
*
      call InitializeAPFEL
```

- If APFEL has not been linked, a dummy file (`apfel_dum.f`) is compiled in place of `apfel.f`.

DGLAP Evolution

The Implementation

- When actually performing the evolution (`evolution.f`), the QCDNUM evolution must be skipped:

```
C ---- APFEL ----
      if (IPDFSET.eq.7) return
```

- However, APFEL should be able to deal with all the PDF decompositions available in HERAFitter.

- Therefore, at the bottom of `evolution.f` there is the subroutine:

```
**********************************************************************
*
*     Subroutine that defines the PDFs to be evolved with APFEL.
*     (predefined name)
*
**********************************************************************
      subroutine ExternalSetAPFEL(x,xf)
```

which, for any given x and for any PDF decomposition, transforms the initial scale PDFs in a format suitable to be fed to APFEL for the evolution.

DGLAP Evolution

The Implementation

- The (x,Q) grid for PDFs is filled in `fcn.f`. Here also the reference value of alphas at the Z mass is set:

```
      if(itheory.eq.0.or.itheory.eq.10) then
         if (itheory.eq.0) then
            call setalf(dble(alphas),Mz*Mz)
         else
            call SetAlphaQCDRef(dble(alphas),dble(Mz))
         endif
         alphaSzero= hf_get_alphas(1D0)
         call RT_SetAlphaS(alphaSzero)
         if(IPDFSET.eq.5) then
            call PDFINP(LHAPDFsubr, IPDFSET, dble(0.001), epsi, nwds)
         elseif (IPDFSET.eq.7) then
            q2p = starting_scale
            call SetPDFSet(“external")
            call PDFINP(APFELsubr,  IPDFSET, dble(0.001), epsi, nwds)
         endif
      endif
```

Set reference value of alphas with QCDNUM or APFEL

fill the (x,Q) grid with LHAPDF or APFEL

- Where the `APFELsubr`, that evolves PDFs using APFEL, is defined in `init_theory.f`:

```
      Subroutine APFELsubr(x, qmu2, xf)
```

DGLAP Evolution

The Implementation

- In order to use the APFEL evolution also for alphas used in the computation of the structure functions, we needed to modify also the `interfaces/src/hf_pdf_calls.f` file:

```
      if (itheory.eq.10) then
         HF_Get_alphas = alphaQCD(dsqrt(q2))
      else
         HF_Get_alphas = ASFUNC(q2,nf,ierr)
      endif
```

APFEL

QCDNUM

- Remark: upon Voica's suggestion and in order to maintain the possibility to run HERAFitter without having LHAPDF installed, we have modified APFEL in such a way that it is now possible to compile it without liking LHAPDF.

- To do so, one just needs to configure APFEL with the flag:

```
./configure --disable-lhapdf
```

DGLAP Evolution

Testing the Code

- Fits using APFEL as a PDF evolver on a reduced subsets of HERA data have been successfully performed leading to results almost identical to those obtained with QCDNUM:

QCDNUM evolution (TheoryType = DGLAP)

```
Dataset    1    106.70   145  NC cross section HERA-I H1-ZEUS combined e-p.
Dataset    2    419.12   379  NC cross section HERA-I H1-ZEUS combined e+p.
Dataset    3     19.87    34  CC cross section HERA-I H1-ZEUS combined e-p.
Dataset    4     29.47    34  CC cross section HERA-I H1-ZEUS combined e+p.
```

APFEL evolution (TheoryType = DGLAP_APFEL)

```
Dataset    1    106.71   145  NC cross section HERA-I H1-ZEUS combined e-p.
Dataset    2    419.16   379  NC cross section HERA-I H1-ZEUS combined e+p.
Dataset    3     19.85    34  CC cross section HERA-I H1-ZEUS combined e-p.
Dataset    4     29.54    34  CC cross section HERA-I H1-ZEUS combined e+p.
```

- The performance, although the implementation is not fully optimal for APFEL, is essentially the same as QCDNUM with some room for possible improvements.

FONLL Structure Functions

The Usage

- APFEL implements also the computation of the FONLL structure functions (used in the NNPDF fits) up to NNLO (FONLL was the only missing scheme in HERAFitter).

- Interface the DIS module of APFEL to HERAFitter in order to fit PDFs in the FONLL scheme.

- Nine new options in the steering card for `HF_scheme`:

```
! ---  HF_SCHEME = 'FONLL-A'          : FONLL-A mass scheme provided by APFEL with pole masses (available only at NLO)
! ---  HF_SCHEME = 'FONLL-A RUNM OFF' : FONLL-A mass scheme provided by APFEL with MSbar masses running OFF (available only at NLO)
! ---  HF_SCHEME = 'FONLL-A RUNM ON'  : FONLL-A mass scheme provided by APFEL with MSbar masses running ON (available only at NLO)
! ---  HF_SCHEME = 'FONLL-B'          : FONLL-B mass scheme provided by APFEL with pole masses (available only at NLO)
! ---  HF_SCHEME = 'FONLL-B RUNM OFF' : FONLL-B mass scheme provided by APFEL with MSbar masses running OFF (available only at NLO)
! ---  HF_SCHEME = 'FONLL-B RUNM ON'  : FONLL-B mass scheme provided by APFEL with MSbar masses running ON (available only at NLO)
! ---  HF_SCHEME = 'FONLL-C'          : FONLL-C mass scheme provided by APFEL with pole masses (available only at NNLO)
! ---  HF_SCHEME = 'FONLL-C RUNM OFF' : FONLL-C mass scheme provided by APFEL with MSbar masses running OFF (available only at NNLO)
! ---  HF_SCHEME = 'FONLL-C RUNM ON'  : FONLL-C mass scheme provided by APFEL with MSbar masses running ON (available only at NNLO)
```

- They correspond to the three variants of the FONLL scheme (A, B and C) with pole and MSbar heavy quark masses (running ON and OFF).

- Since QCDNUM does not implement the VFNS evolution with MSbar masses, the options above should be used only with the APFEL evolution.

FONLL Structure Functions

The Implementation

- Like all other heavy quark schemes, the FONLL scheme is initialized in `init_theory.f`:

```
      if (mod(HFSCHEME,10).eq.3) then
         Call FF_init()
      elseif ( mod(HFSCHEME,10).eq.2) then
         Call RT_Init()
      elseif ( mod(HFSCHEME,10).eq.4) then
         Call ABKM_init()
      elseif ( mod(HFSCHEME,10).eq.5) then
         Call FONLL_init()
      endif
```

- and the corresponding cross sections computed in `dis_sigma.f`:

```
         elseif (mod(local_hfscheme,10).eq.5) then
            call UseFONLLScheme(F2,FL,xF3,F2c,FLc,F2b,FLb,
     1                          x,q2,npts,polarity,XSecType,
     2                          charge,local_hfscheme,IDataSet)
```

- All the new routines needed to initialize and compute the FONLL structure functions with APFEL are in the new `FONLL` subdirectory placed in the main HERAFitter folder.

FONLL Structure Functions

Results: Pole Masses

- TR scheme at NLO

```
                    399      575.08   582        0.99
After minimisation     575.08   582     0.988
Dataset    1    106.70   145  NC cross section HERA-I H1-ZEUS combined e-p.
Dataset    2    419.12   379  NC cross section HERA-I H1-ZEUS combined e+p.
Dataset    3     19.84    34  CC cross section HERA-I H1-ZEUS combined e-p.
Dataset    4     29.42    34  CC cross section HERA-I H1-ZEUS combined e+p.
 Correlated Chi2    0.0000000000000000
 --------- in store-pdfs -------
cpu_time    353.77    354.27      0.50
```

- FONLL-A scheme (NLO)

```
                   1033      566.82   582        0.97
After minimisation     566.82   582     0.974
Dataset    1    107.61   145  NC cross section HERA-I H1-ZEUS combined e-p.
Dataset    2    409.35   379  NC cross section HERA-I H1-ZEUS combined e+p.
Dataset    3     19.99    34  CC cross section HERA-I H1-ZEUS combined e-p.
Dataset    4     29.86    34  CC cross section HERA-I H1-ZEUS combined e+p.
 Correlated Chi2    0.0000000000000000
 --------- in store-pdfs -------
cpu_time    625.82    626.28      0.45
```

- FONLL-B scheme (NLO)

```
                    795      547.20   582        0.94
After minimisation     547.20   582     0.940
Dataset    1    107.95   145  NC cross section HERA-I H1-ZEUS combined e-p.
Dataset    2    388.86   379  NC cross section HERA-I H1-ZEUS combined e+p.
Dataset    3     20.25    34  CC cross section HERA-I H1-ZEUS combined e-p.
Dataset    4     30.15    34  CC cross section HERA-I H1-ZEUS combined e+p.
 Correlated Chi2    0.0000000000000000
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cpu_time    482.09    482.55      0.47
```

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Improvement of the chi2
(especially for FONLL-B)

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Improvement of the chi2 (especially for FONLL-B)

the FONLL scheme (i.e. APFEL) is substantially faster than TR: (0.6 vs. 0.9 s per iteration)

FONLL Structure Functions

Results: Pole Masses

- TR scheme at NNLO

```
                    1268      637.91   582        1.10
After minimisation     637.91   582     1.096
Dataset    1    107.27   145  NC cross section HERA-I H1-ZEUS combined e-p.
Dataset    2    474.98   379  NC cross section HERA-I H1-ZEUS combined e+p.
Dataset    3     19.55    34  CC cross section HERA-I H1-ZEUS combined e-p.
Dataset    4     36.11    34  CC cross section HERA-I H1-ZEUS combined e+p.
 Correlated Chi2    0.0000000000000000
 --------- in store-pdfs -------
cpu_time   2061.71   2062.19      0.49
```

- FONLL-C scheme (NNLO)

```
                    1284      619.74   582        1.06
After minimisation     619.74   582     1.065
Dataset    1    105.63   145  NC cross section HERA-I H1-ZEUS combined e-p.
Dataset    2    460.51   379  NC cross section HERA-I H1-ZEUS combined e+p.
Dataset    3     19.43    34  CC cross section HERA-I H1-ZEUS combined e-p.
Dataset    4     34.16    34  CC cross section HERA-I H1-ZEUS combined e+p.
 Correlated Chi2    0.0000000000000000
 --------- in store-pdfs -------
cpu_time    819.16    819.64      0.48
```

FONLL Structure Functions

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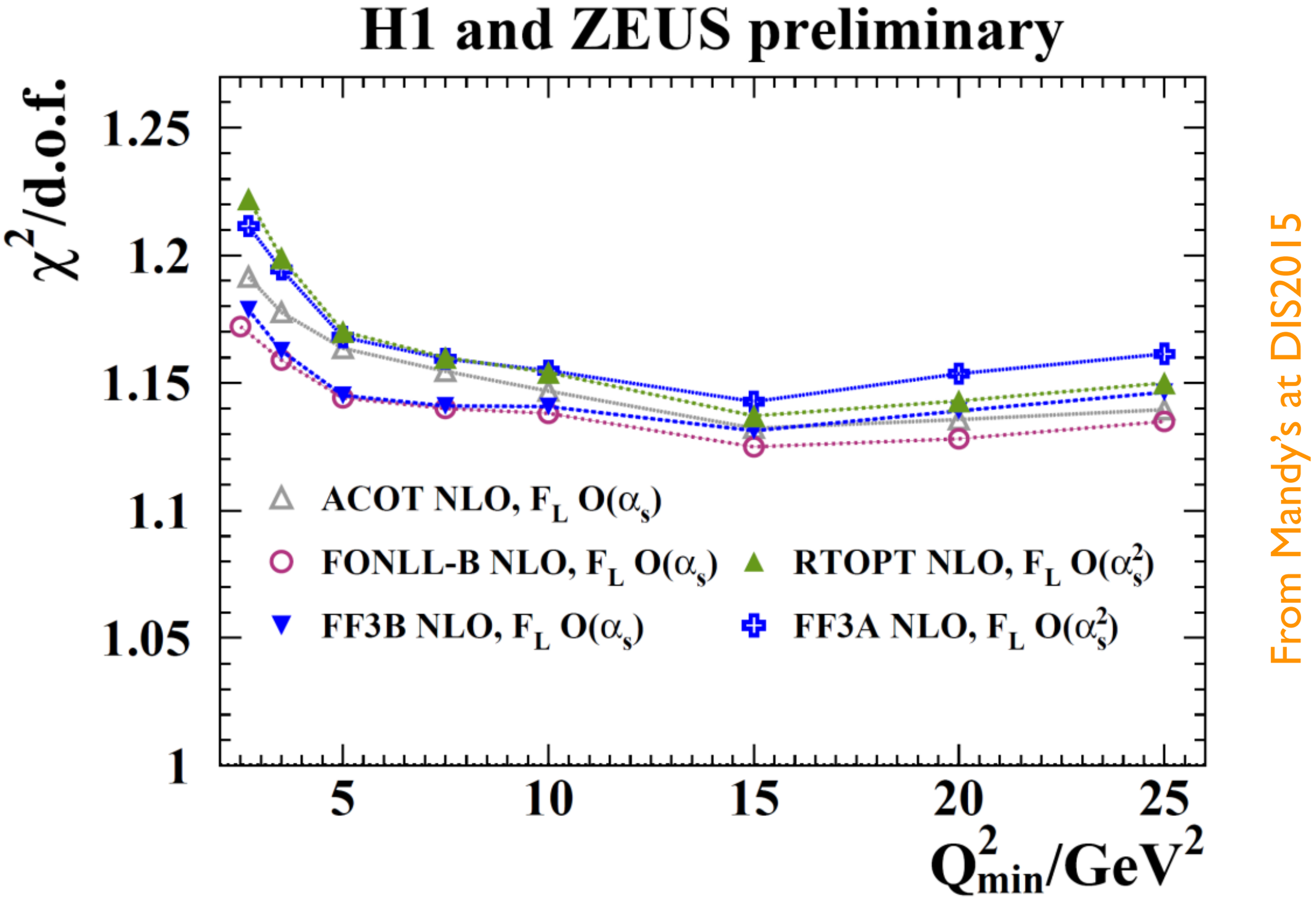
the FONLL scheme (i.e. APFEL) is substantially faster than TR: (0.64 vs. 1.6 s per iteration)

FONLL Structure Functions

Results: Pole Masses



From Mandy's at DIS2015

FONLL Structure Functions

Results: MSbar Masses

- Preliminary tests using the default parameters of HERAfitter (*i.e.* numerical values of the pole masses):
  - FONLL-B scheme (NLO) with pole masses:

```
After minimisation     547.21   582     0.940
Dataset    1    107.95   145  NC cross section HERA-I H1-ZEUS combined e-p.
Dataset    2    388.85   379  NC cross section HERA-I H1-ZEUS combined e+p.
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Dataset    4     30.17    34  CC cross section HERA-I H1-ZEUS combined e+p.
```

  - FONLL-B scheme (NLO) with MSbar masses (running OFF)

```
After minimisation     545.07   582     0.937
Dataset    1    108.09   145  NC cross section HERA-I H1-ZEUS combined e-p.
Dataset    2    387.00   379  NC cross section HERA-I H1-ZEUS combined e+p.
Dataset    3     20.07    34  CC cross section HERA-I H1-ZEUS combined e-p.
Dataset    4     29.91    34  CC cross section HERA-I H1-ZEUS combined e+p.
```

  - FONLL-B scheme (NLO) with MSbar masses (running ON)

```
After minimisation     539.90   582     0.928
Dataset    1    108.39   145  NC cross section HERA-I H1-ZEUS combined e-p.
Dataset    2    381.68   379  NC cross section HERA-I H1-ZEUS combined e+p.
Dataset    3     20.13    34  CC cross section HERA-I H1-ZEUS combined e-p.
Dataset    4     29.70    34  CC cross section HERA-I H1-ZEUS combined e+p.
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FONLL Structure Functions

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Dataset    3     20.13     34  CC cross section HERA-I H1-ZEUS combined e-p.
Dataset    4     29.70     34  CC cross section HERA-I H1-ZEUS combined e+p.
```

Improvement of the χ^2 in the MSbar scheme, more pronounced when considering the running of the masses.

⇩

need for a more detailed study

- Similar results in the FONLL-C scheme (NNLO).

Interfacing APFEL to HERAFitter

Conclusions and Outlook

- APFEL has been "fully" interfaced to HERAFitter which now benefits of the evolution and the FONLL structure functions both with pole and MSbar masses.

- The FONLL scheme seems to provide a good description of the HERA data and preliminary tests show that the use of the MSbar masses might provide a further improvement.

- Next steps to be taken are:

  - implementation of the coupled QCD+QED evolution and fit of the photon PDFs,

  - …