The evolution of APFEL: APFEL++

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Motivation

- Since its born, APFEL has undergone a large number of developments:
  - FONLL structure functions,
  - NLO QED evolution,
  - lepton PDFs,
  - Scale variations,
  - intrinsic charm,
  - displaced thresholds,
  - MS masses,
  - small-x resummation,
  - interface to the NNPDF code,
  - …
- Way beyond the purposes for which it was conceived:
  - very large memory footprint,
  - non-optimal "convenience" solutions for the new modules,
  - hard to maintain.
- APFEL is written in FORTAN77 that is not suitable for large projects:
  - lack of modularity,
  - non-optimal (built-in) memory management.
- Compelling reasons to rewrite APFEL keeping in mind its applications.

Design of the code

- Concerning the **language**, **C++** was a somewhat natural choice:
  - **modularity** ensured by the object-oriented nature,
  - **dynamical** allocation of the **memory**,
  - used for the new-generation tools (*e.g.* LHAPDF) and thus easier **interface**,
  - powerful features coming with the **C++11 standard**.
- The code **design** was driven by a profound rethinking of the strategy:
  - the main application field is **collinear factorisation**.
  - In this context, most of the relevant quantities are computed as **convolutions**:

$$M(x) = \int_x^1 \frac{dy}{y} O(y) d\left(\frac{x}{y}\right) = \int_x^1 \frac{dz}{z} O\left(\frac{x}{z}\right) d(z) \equiv O(x) \otimes d(x)$$

operator O: typically a complicated object slow to compute: *e.g.* a **perturbative** hard cross section.
distribution d: typically a fast-to-access function: *e.g.* a **non-perturbative** PDF or a FF.

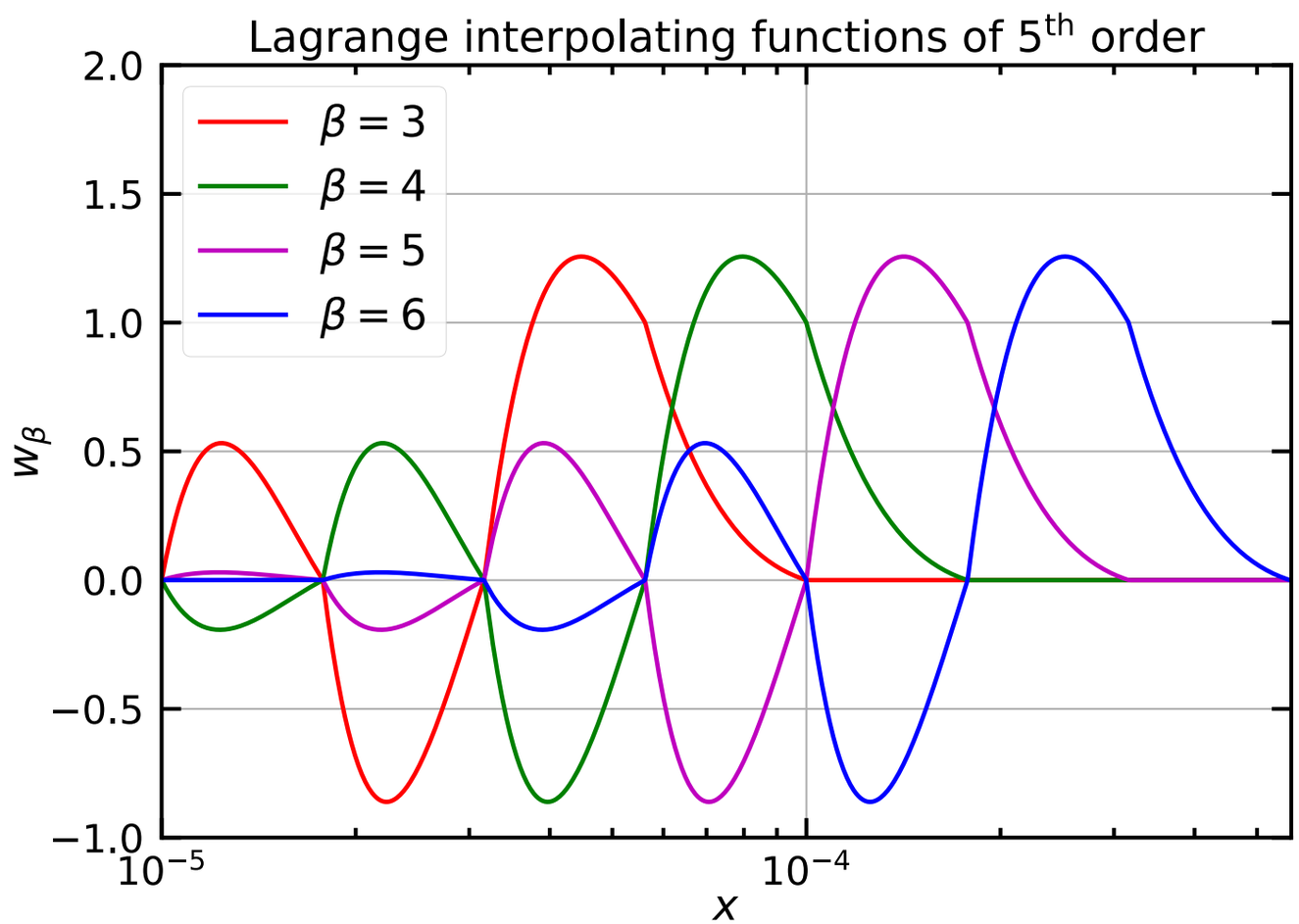
  - Adopt the ***x*-space** (as opposed to N-space) formalism:
    - most of the results are available in x-space,
    - no restriction on the parameterisations.
  - The purpose is to make convolutions **fast**.

Design of the code

- Define an **interpolation grid** in x with N+1 nodes $g \equiv \{z_0, \ldots, z_N\}$
- Use the interpolation formula for the **distribution** d:

$$d(z) = \sum_{\beta=0}^{N} w_\beta(z) d_\beta \quad \text{with} \quad d_\beta = d(x_\beta)$$

  - $w_\beta(z)$ *interpolating function* (typically a Lagrange polynomial of some degree ***n***).



  - **piecewise** function different from zero over ***n + 1*** intervals around ***β***. **Zero** elsewhere. **Hard to integrate**.

Design of the code

- Compute the integral of the **operator** O with the interp. functions:

$$O_{\alpha\beta} \equiv \int_{x_\alpha}^{1} \frac{dy}{y} O(y) w_\beta \left(\frac{x_\alpha}{y}\right)$$

such that:

$$M_\alpha \equiv \sum_{\beta=0}^{N} O_{\alpha\beta} d_\beta \quad \text{with} \quad M(x) = \sum_{\alpha=0}^{N} w_\alpha(x) M_\alpha$$

- This reduces convolutions to multiplications between a matrices and vectors: **linear algebra**.
- Therefore, the **three main ingredients** of of APFEL++ are:
  1. the **interpolation grid** g along with the interpolating functions,
  2. the **distribution** d_β,
  3. the **operator** $O_{\alpha\beta}$.
- They can be **encapsulated** in **C++ objects** to compute convolutions.

Design of the code

- An additional complication is given by the **flavour structure**:
  - distributions are **vectors in flavour space**,
  - operators are either **matrices or vectors in the flavour space**.

$$\frac{d f_{i\alpha}}{d \ln \mu^2} = \sum_{j,\beta} P^{ij}_{\alpha\beta} f_{j\beta}$$

DGLAP equations

$$F_\alpha = \sum_{j,\beta} C^{j}_{\alpha\beta} f_{j\beta}$$

DIS structure functions

- Matrices in flavour space are often **sparse**.
- Define **sets of objects** with a **flavour map**:
  - associate one operator to one distribution, *e.g.*:

$$\begin{array}{lcl} P_{qq}, P_{gq} & \to & \Sigma \\ P_{qg}, P_{gg} & \to & g \\ P^v & \to & V \\ P^+ & \to & T_{3,8,15,24,35} \\ P^- & \to & V_{3,8,15,24,35} \end{array}$$

    - the same operator can be assigned to more than a distribution and viceversa.
  - avoid **multiplications by zero**.

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Set of operators	Flavour map	Set of distributions
P_{qq}, P_{gq}	$\rightarrow$	Σ
P_{qg}, P_{gg}	$\rightarrow$	g
P^v	$\rightarrow$	V
P^+	$\rightarrow$	$T_{3,8,15,24,35}$
P^-	$\rightarrow$	$V_{3,8,15,24,35}$

    - the same operator can be assigned to more than a distribution and viceversa.
  - avoid **multiplications by zero**.

Design of the code

- Define **multiplication** between sets of distributions and operators:
  - **overload** multiplication operator in C++.
  - Making convolutions with a flavour structure becomes very **easy**.

```
//_____________________________________________________________________________
Set<Distribution> Dglap::Derivative(int const& nf, double const& t, Set<Distribution> const& f) const
{
  return _SplittingFunctions(nf, exp(t/2)) * f;
}
```

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```

Set of operators

Set of distributions

Overloaded multiplication:
takes care of convolutions
and flavour structure

- The flavour structure is completely defined by the flavour map:
  - **same procedure** for convolutions in **any flavour basis**,
  - sets of operators and distributions multiplied only if they **share** the same map,
  - easy to account for n_f **dependence**.

Design of the code

- Use (e.g.) 4th order Runge-Kutta to solve systems of **ordinary differential equations:**

$$\begin{cases} \dfrac{d\mathbf{y}}{dt} = \mathbf{F}(t, \mathbf{y}) \\ \\ \mathbf{y}(t_0) = \mathbf{y}_0 \end{cases}$$

Template function…
… that returns a **std::function**…
… of a **std::function**

Five nested **Lambda** functions

```
template<class U>
function<U(double const&, U const&, double const&)>
rk4(function<U(double const& t, U const& Obj)> const& f)
{
  return
    [       f              ](double const& t, U const& y,  double const& dt) -> U{ return
    [t,y,dt,f              ](                 U const& dy1                  ) -> U{ return
    [t,y,dt,f,dy1          ](                 U const& dy2                  ) -> U{ return
    [t,y,dt,f,dy1,dy2      ](                 U const& dy3                  ) -> U{ return
    [t,y,dt,f,dy1,dy2,dy3](                 U const& dy4                  ) -> U{ return
    ( dy1 + 2 * dy2 + 2 * dy3 + dy4 ) / 6  ;} (
    dt * f( t + dt     , y + dy3     )     );} (
    dt * f( t + dt / 2, y + dy2 / 2 )     );} (
    dt * f( t + dt / 2, y + dy1 / 2 )     );} (
    dt * f( t          , y           )     );} ;
}
```

- Very same function used to solve **both** the DGLAP and the α_s RGE.

Doxygen documentation

https://vbertone.github.io/apfelxx/html/index.html

vbertone.github.io

Google CERN Account VUnet DFS webpages Wiki arXiv Inspire WordReference Mijn Belastingdienst La Repubblica Il Fatto Quotidiano Flightradar24 Vidyo ATLAS Results CMS Results

APFEL++ APFEL 4.0.0

A PDF evolution library in C++

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APFEL Documentation

APFEL++

APFEL++: A new PDF evolution library in C++

APFEL++ is a C++ rewriting of the Fortran 77 evolution code APFEL (see http://apfel.hepforge.org and https://github.com/scarrazza/apfel). APFEL++ is based on a completely new code design and guarantees a better performance along with a more optimal memory management. The new modular structure allows for a better maintainability and an easier extensibility. This makes APFEL++ suitable for a wide range of tasks: from the solution of the DGLAP evolution equations to the computation of deep-inelastic-scattering (DIS) and single-inclusive-annihilation cross sections. Also more complex computations, like semi-inclusive DIS and Drell-Yan cross sections, are easily implementable in APFEL++.

Download

You can obtain APFEL++ directly from the github repository:

https://github.com/vbertone/apfelxx/releases

For the last development branch you can clone the master code:

```
git clone https://github.com/vbertone/apfelxx.git
```

Modules

Here is a list of all modules:

- DIS convolution maps
- Evolution convolution maps
- Recurrent expressions
- ▼ Massless limit of the massive neutral current coefficient functions
  - LO massive-zero coefficient functions
  - NLO massive-zero coefficient functions
- Matching convolution maps
- ▼ Space-like matching conditions
  - NLO matching conditions
  - NNLO matching conditions
- ▼ Time-like matching conditions
  - NLO matching conditions
- ▼ TMD matching functions
  - ▼ Space-like matching functions
    - NLO matching functions for PDFs
    - NNLO matching functions for PDFs
  - ▼ Time-like matching functions
    - NLO matching functions for FFs
    - NNLO matching functions for FFs
- ▼ Space-like splitting function
  - ▼ Unpolarised splitting functions

Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

[detail level 1 2 3]

▼ N apfel	Namespace for all APFEL++ functions and classes
C AlphaQCD	The AlphaQCD is a specialization class of the MatchedEvolution class for the computation of the QCD coupling running
C ANS2qqH_0	$O(\alpha_s^2)$ constant term of eq (B.4) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C ANS2qqH_L	$O(\alpha_s^2)$ term propotional to $\ln(\mu^2/m^2)$ of eq (B.4) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C ANS2qqH_L2	$O(\alpha_s^2)$ term propotional to $\ln^2(\mu^2/m^2)$ of eq (B.4) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C APS2Hq_0	$O(\alpha_s^2)$ constant term of eq (B.1) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C APS2Hq_L	$O(\alpha_s^2)$ term propotional to $\ln(\mu^2/m^2)$ of eq (B.1) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C APS2Hq_L2	$O(\alpha_s^2)$ term propotional to $\ln^2(\mu^2/m^2)$ of eq (B.1) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C AS1ggH_L	$O(\alpha_s)$ term propotional to $\ln(\mu^2/m^2)$ of eq (B.6) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C AS1Hg_L	$O(\alpha_s)$ term propotional to $\ln(\mu^2/m^2)$ of eq. (B.2) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C AS2ggH_0	$O(\alpha_s^2)$ constant term of eq (B.7) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C AS2ggH_L	$O(\alpha_s^2)$ term propotional to $\ln(\mu^2/m^2)$ of eq (B.7) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C AS2ggH_L2	$O(\alpha_s^2)$ term propotional to $\ln^2(\mu^2/m^2)$ of eq (B.7) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C AS2gqH_0	$O(\alpha_s^2)$ constant term of eq (B.5) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C AS2gqH_L	$O(\alpha_s^2)$ term propotional to $\ln(\mu^2/m^2)$ of eq (B.5) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C AS2gqH_L2	$O(\alpha_s^2)$ term propotional to $\ln^2(\mu^2/m^2)$ of eq (B.5) of https://arxiv.org/pdf/hep-ph/9612398.pdf
C AS2Hg_0	$O(\alpha_s^2)$ constant term of eq (B.3) of https://arxiv.org/pdf/hep-ph/9612398.pdf

Convoluting operators

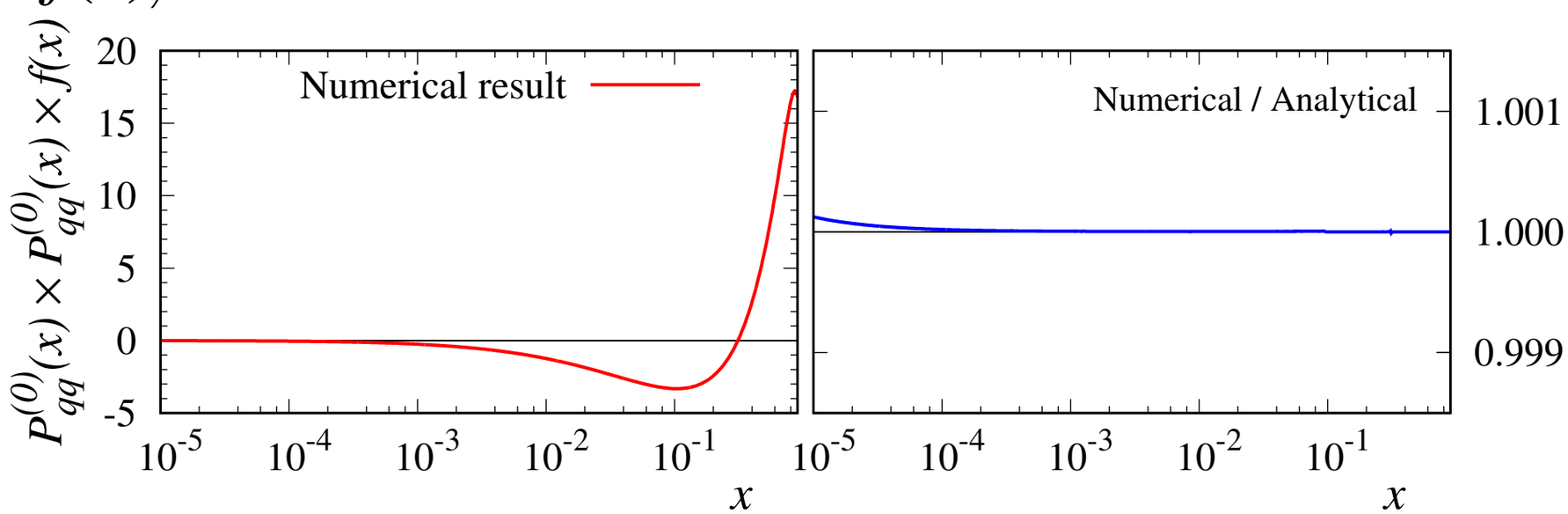
- An operation that is often needed is the convolution between operators:
  - involved in the computation of factorisation **scale variations**,
  - computation of the **PDF evolution operator**.

$$M(x) = \underbrace{O^{(1)}(x) \otimes O^{(2)}(x)}_{O(x)} \otimes d(x) \;\rightarrow\; M_\alpha = \sum_\beta \underbrace{\sum_\gamma O^{(1)}_{\alpha\gamma} O^{(2)}_{\gamma\beta}}_{O_{\alpha\beta}} d_\beta$$

- Consider for example:

$$P^{(0)}_{qq}(x) = \left(\frac{1+x^2}{1-x}\right)_+ \quad \text{such that} \quad \begin{aligned} P^{(0)}_{qq}(x) \otimes P^{(0)}_{qq}(x) &= \left(\frac{4(x^2+1)\ln(1-x)+x^2+5}{1-x}\right)_+ \\ &- \frac{(3x^2+1)\ln x}{1-x} - 4 + \left(\frac{9}{4} - \frac{2\pi^2}{3}\right)\delta(1-x) \end{aligned}$$

- Compare the numerical convolution with the analytic result (using a test function $f(x)$):



Evolution operator

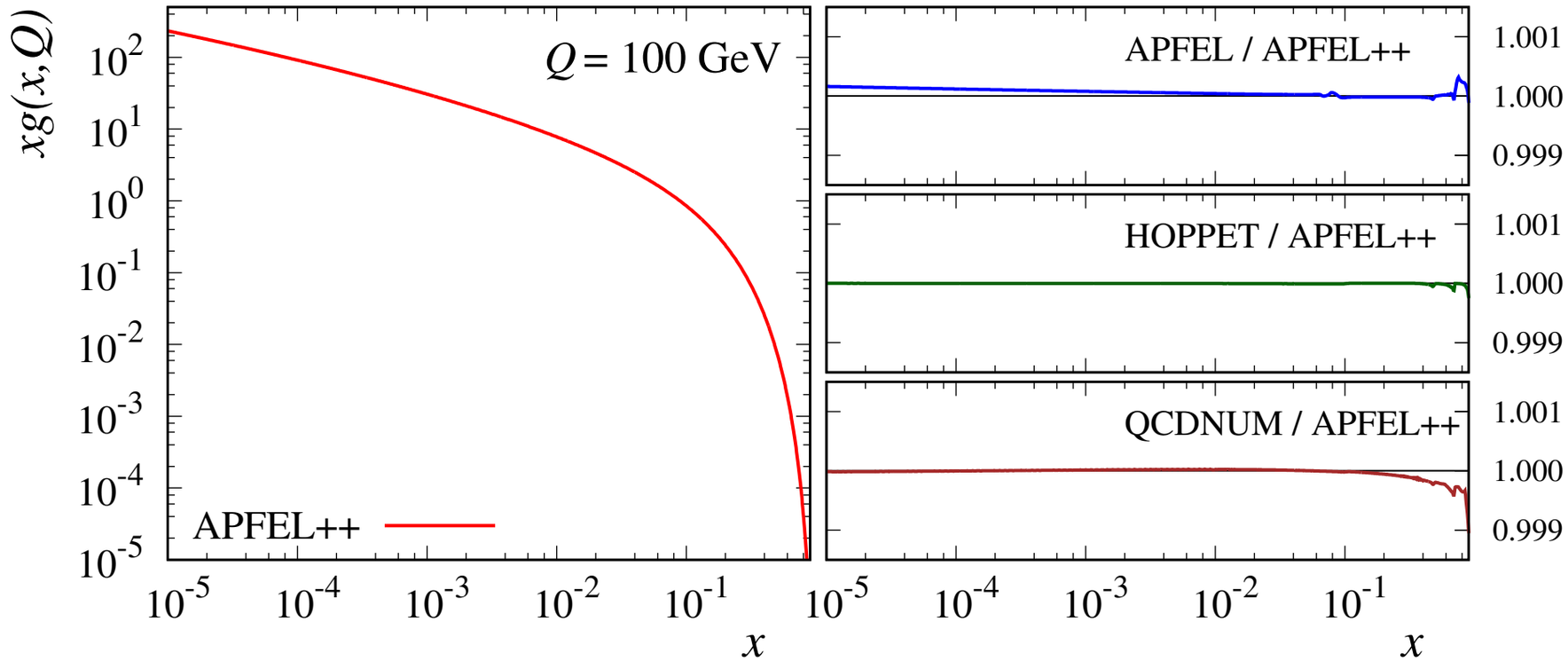
- The DGLAP can be written in terms the **evolution operator**:

$$\begin{cases} \dfrac{d}{d\ln\mu^2}\Gamma^{ij}_{\alpha\beta}(\mu_0,\mu) = \sum_{k,\gamma} P^{ik}_{\alpha\gamma}(\mu)\Gamma^{kj}_{\gamma\beta}(\mu_0,\mu) \\ \\ \Gamma^{ij}_{\alpha\beta}(\mu_0,\mu_0) = \delta_{ij}\delta_{\alpha\beta} \end{cases}$$

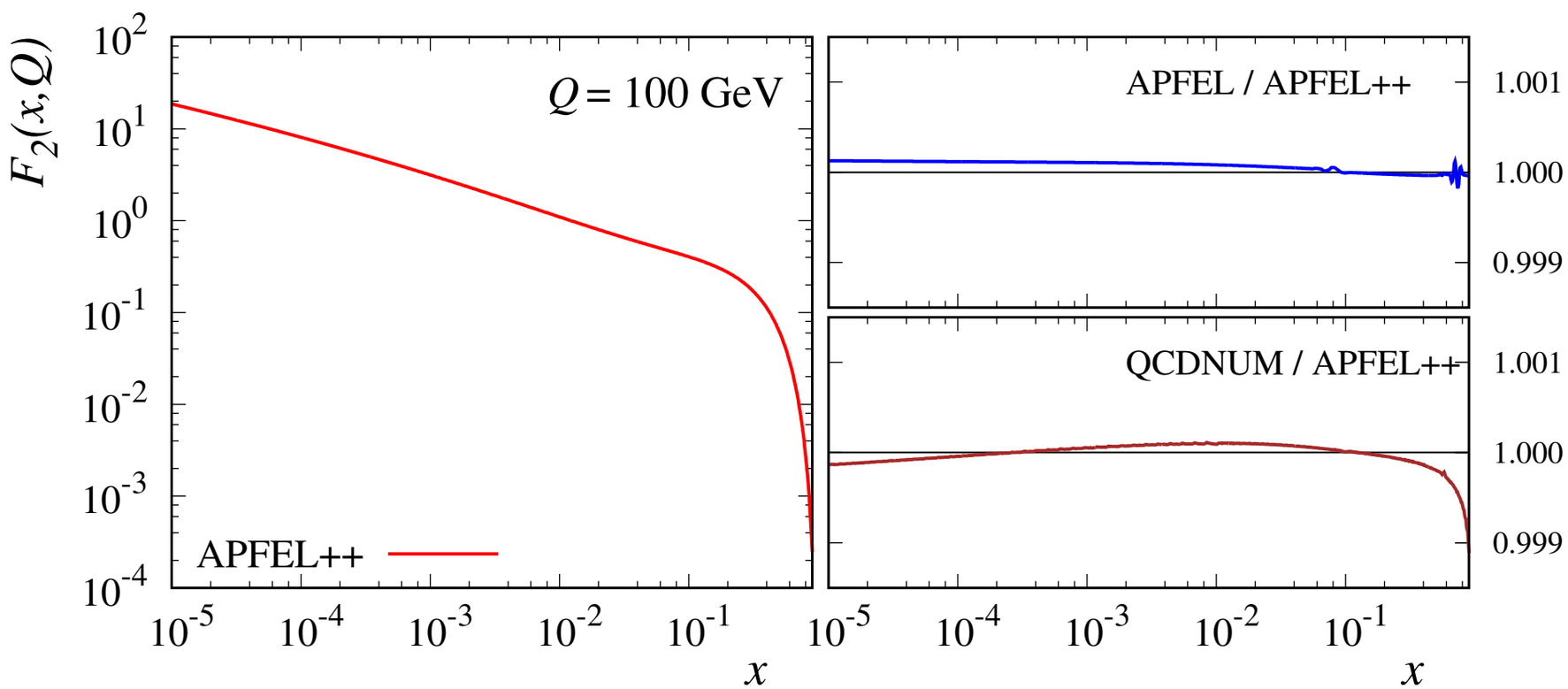
- The evolution operator can be used to evolve any initial scale PDF:
  - **harder** to compute than evolving PDFs,
  - it has to be computed **only once** (for each μ_0 and μ).
- This object is used for the construction of the **APFELgrid** tables:
  - extremely hard to compute in APFEL (Fortran),
  - very easy with APFEL++.

Applications

- DGLAP evolution at NNLO:



- DIS structure functions at NNLO:



PDF evolution performance

- Comparison between different codes:

NNLO QCD evolution ~200 points in x ~50 points in Q	Initialisation [s]	Interpolate PDFs 10^6 times [s]
APFEL++	0.4 (0.27 in. + 0.13 tab.)	0.6
APFEL	2.4	1.9
HOPPET	0.4	1.3
QCDNUM	8.7	1.3

- Compare APFEL++ to LHAPDF when interpolating a **std::map**:

PDF set: NNPDF31_nlo_as_0118	Interpolate a PDF map 10^5 times [s]
APFEL++	0.7
LHAPDF	0.5

Old functionalities

- The FORTRAN version of APFEL implements a **very large** number of functionalities.
- I'm currently working to implement all of them also in APFEL++.
- **Missing** functionalities in APFEL++ to be implemented:
  - QED corrections,
  - intrinsic charm,
  - $\overline{\text{MS}}$ masses,
  - small-x resummation (need to interface APFEL++ to HELL),
  - scale variations,
  - "minor" functionalities:
    - target mass corrections,
    - different solutions for the DGLAP and coupling evolutions (?).

New functionalities

- I have already started using APFEL++ for tasks difficult to implement in (or even out of reach) for the FORTAN version.
- Examples are:
  - Semi-Inclusive DIS (SIDIS) in collinear factorisation:
    - double convolution with time- and space-like evolution at the same time.
  - TMD phenomenology:
    - evolution and matching,
    - Drell-Yan and SIDIS q_T distributions.
  - DGLAP evolution with splitting explicitly depending the factorisation scale:
    - e.g. “Physical”-scheme evolution (by Martin and Ryskin).
  - Transversity distributions (PDFs and FFs).

SIDIS in collinear factorisation

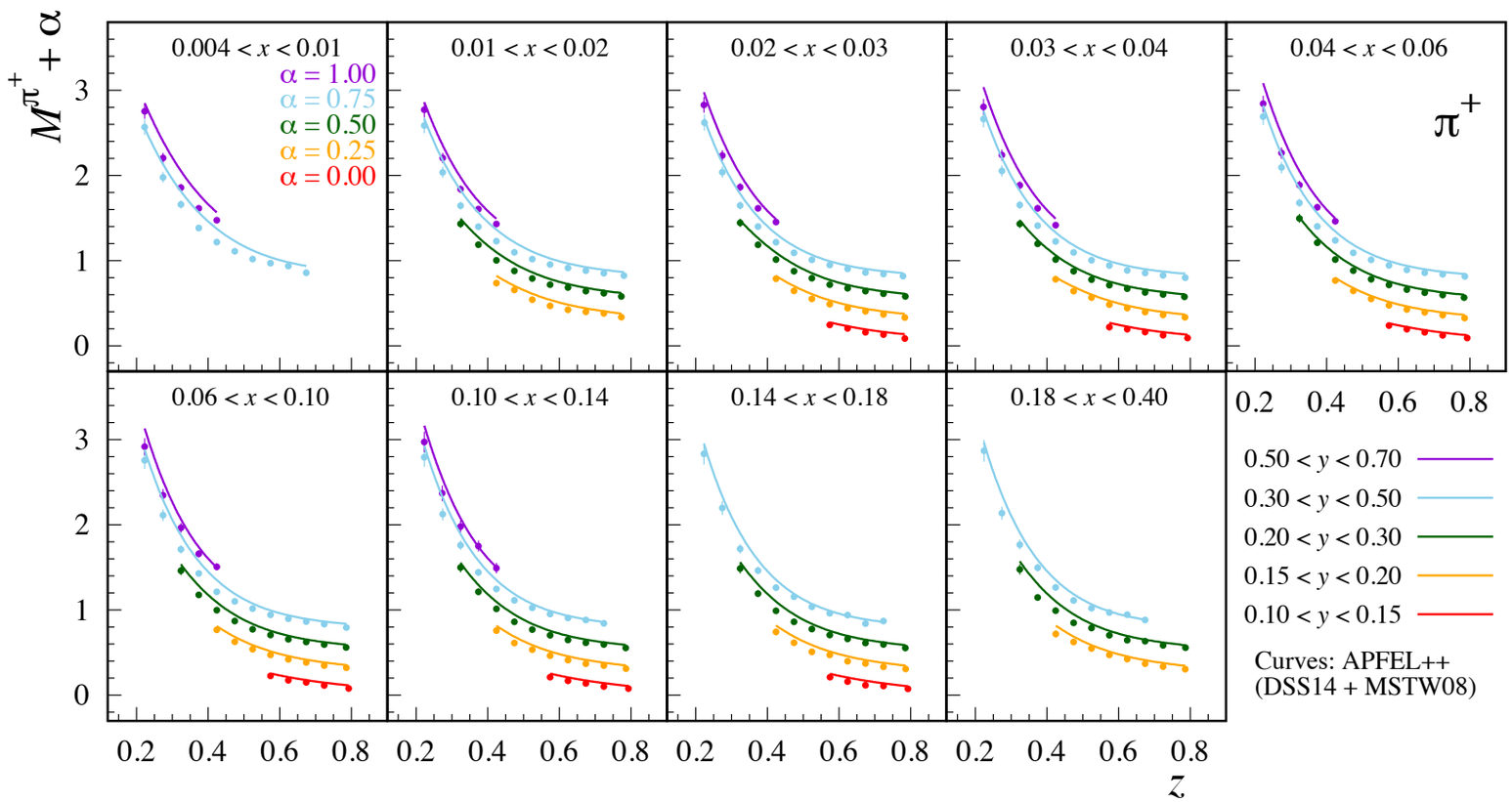
- SIDIS cross sections (integrated over q_T) have this structure:

$$D(x,z) = \int_x^1 \frac{d\xi}{\xi} \int_z^1 \frac{d\zeta}{\zeta} O\left(\frac{x}{\xi}, \frac{z}{\zeta}\right) d^{(1)}(\xi)\, d^{(2)}(\zeta)$$

- But the hard cross sections (at least up to NLO) factorise as:

$$O(x,z) = \sum_i K_i C_i^{(1)}(x) C_i^{(2)}(z)$$

- Combination of single convolutions:



- Next I will also try with Drell-Yan cross sections.

TMD Evolution (PDFs)

$$
\begin{aligned}
F_{f/P}(x, \mathbf{b}_T; \mu, \zeta) &= \sum_j C_{f/j}(x, b_*; \mu_b, \zeta_F) \otimes f_{j/P}(x, \mu_b) && : A \\
&\times \exp\left\{ K(b_*; \mu_b) \ln \frac{\sqrt{\zeta_F}}{\mu_b} + \int_{\mu_b}^{\mu} \frac{d\mu'}{\mu'} \left[\gamma_F - \gamma_K \ln \frac{\sqrt{\zeta_F}}{\mu'} \right] \right\} && : B \\
&\times \exp\left\{ g_{j/P}(x, b_T) + g_K(b_T) \ln \frac{\sqrt{\zeta_F}}{\sqrt{\zeta_{F,0}}} \right\} && : C
\end{aligned}
$$

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$$\times \exp\left\{ g_{j/P}(x, b_T) + g_K(b_T) \ln \frac{\sqrt{\zeta_F}}{\sqrt{\zeta_{F,0}}} \right\} \quad : C$$

- $b_T \ll 1/\Lambda_{QCD}$
- matching to the collinear region
- factorises as hard and non-perturbative
- numerically cumbersome
- precompute using APFEL

- CS evolution
- perturbative

- matching between the small and large b_T
- non perturbative
- parametrised and fitted to data

SIDIS in TMD factorisation

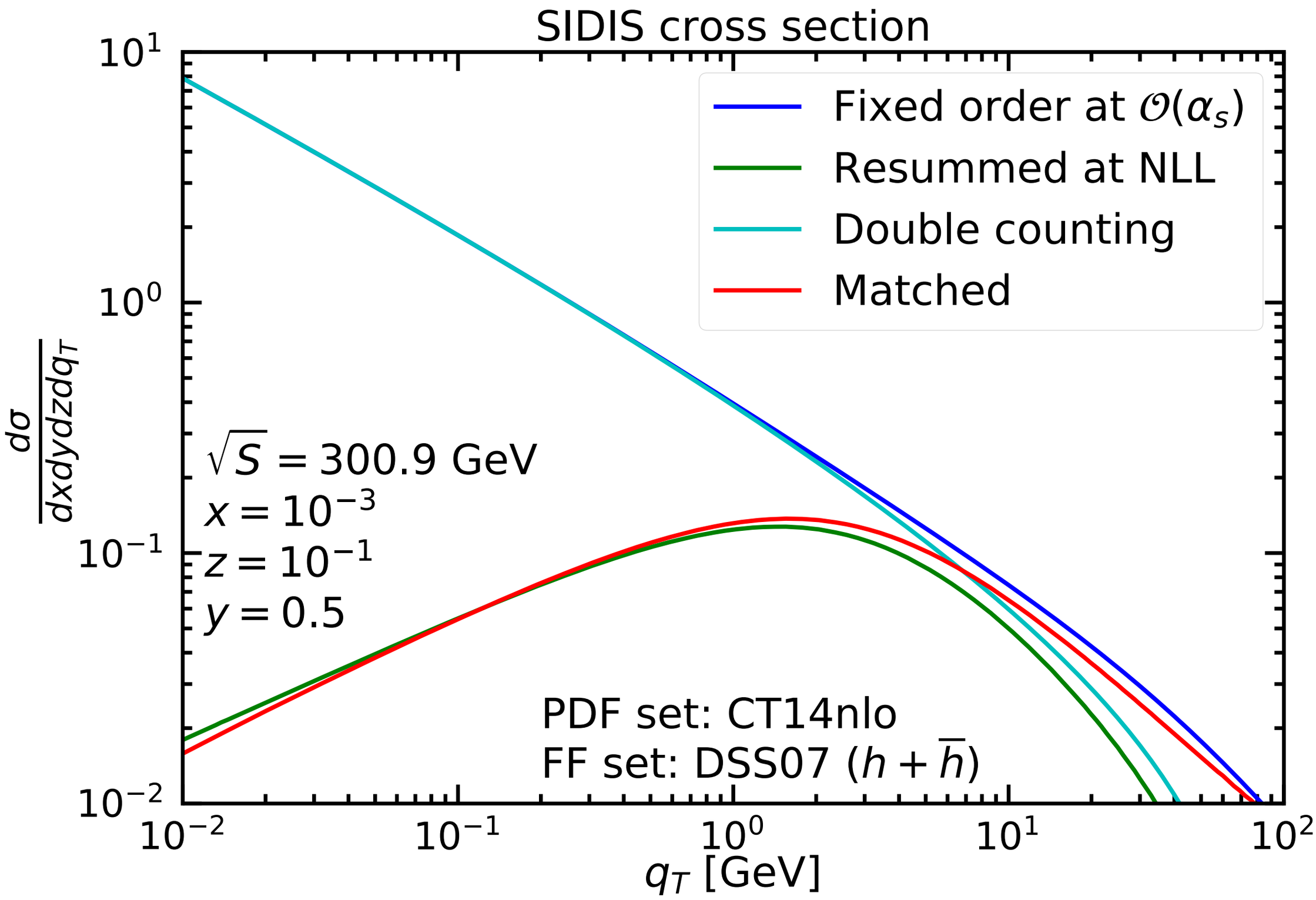
- In SIDIS, what enters the computation of the cross sections is:

$$\mathcal{L}_{\rm SIDIS} = \int \frac{d^2\mathbf{b}_T}{(2\pi)^2} e^{-i\mathbf{q}_T\cdot\mathbf{b}_T} F_{f/P}(x,\mathbf{b}_T;\mu,\zeta_F) D_{H/f}(x,\mathbf{b}_T;\mu,\zeta_D)$$

Fourier transform PDFs FFs

- The ingredients are:
  - a set of evolved TMD-PDFs,
  - a set of evolved TMD-FFs,
  - the Fourier transform of its product.
- Complex set of tasks that have to be performed optimally
- APFEL provides the ideal environment for this computation:
  - fast and accurate interpolation techniques,
  - precomputation of the time consuming bits.

Matching collinear and TMD regimes



Plans for the future

- High-level user interface:
  - set of functions to access the various functionalities,
  - ensure back-compatibility with APFEL?
- Interface to LHAPDF:
  - create with APFEL objects to be fed to LHAPDF,
  - LHAPDF takes care of doing the interpolation,
  - "standard" interface commonly used in our field.
- Interface to yaml for parsing of evolution parameters.
- Interface to APFELgrid.
- Interface to APPLgrid/FastNLO:
  - Drell-Yan and SIDIS cross sections (?).
- PDF evol. and structure functions in a "OO" fashion useful for **xFitter**:
  - many possible evolution and structure functions available at the same time,
  - assign different evolutions to different datasets (e.g. H-VFNS),
  - fit PDFs and FFs at the same time (space- and time-like evolution).