The evolution of APFEL: APFEL++

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3DSPIN
MAPPING THE PROTON IN 3D

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,
  - $\overline{\rm MS}$ 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 FORTRAN77 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++11/17 standard**.
- The code **design** was driven by a profound rethinking of the strategy:
  - the main application field is **collinear/TMD factorisation**.
  - In this context, many 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.

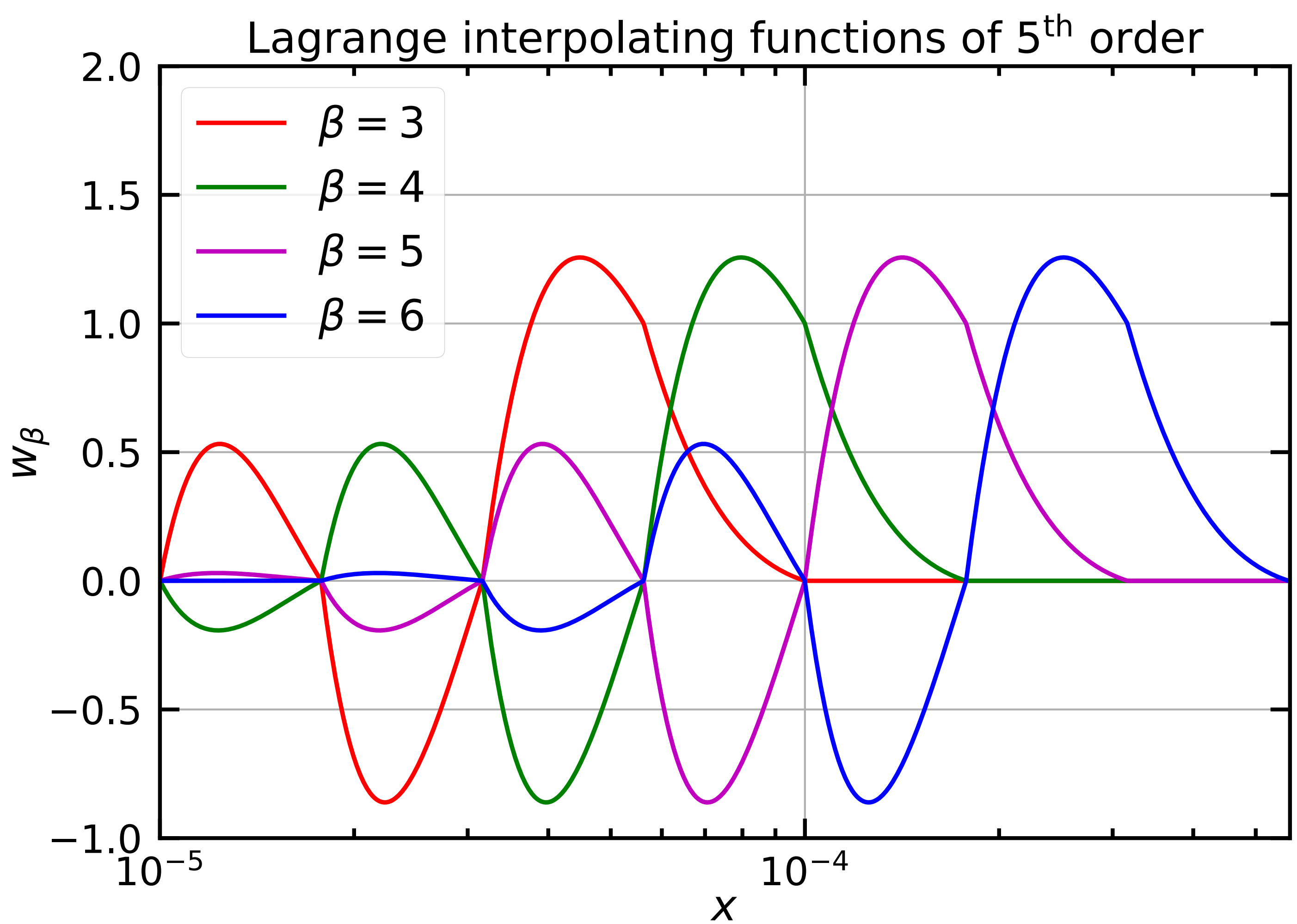
  - Adopt the ***x*-space** (as opposed to *N*-space) formalism:
    - most of the results are available in *x*-space,
    - no restriction on the parameterisations.
  - The purpose is to make convolutions **fast**.

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 $\boldsymbol{n}$).



  - **piecewise** function different from zero over $\boldsymbol{n+1}$ intervals around $\boldsymbol{\beta}$. **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**.

Design of the code

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

DGLAP equations

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

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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 distributions

Set of operators

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**

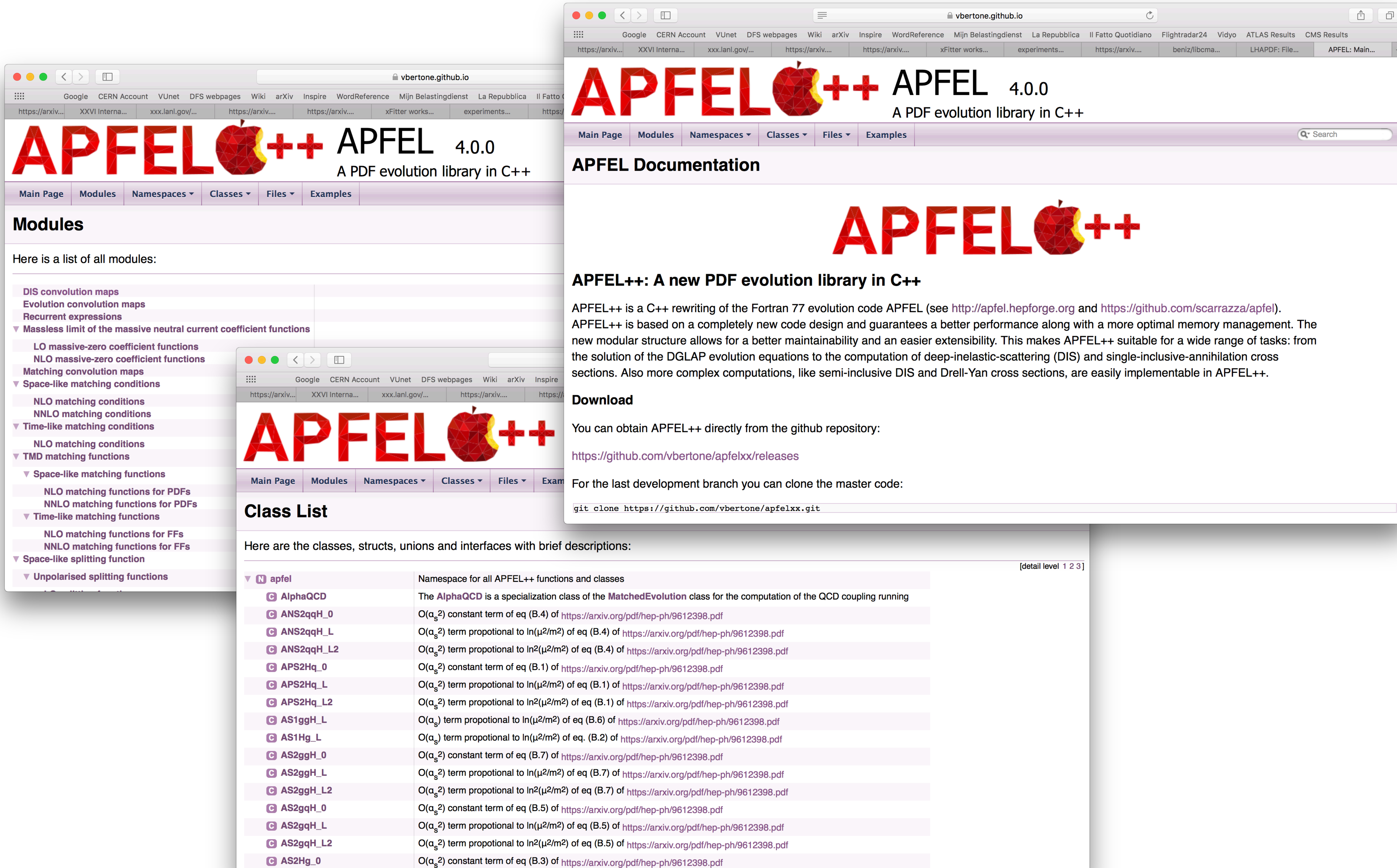
Five nested **Lambda** functions

```
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



Convoluting operators

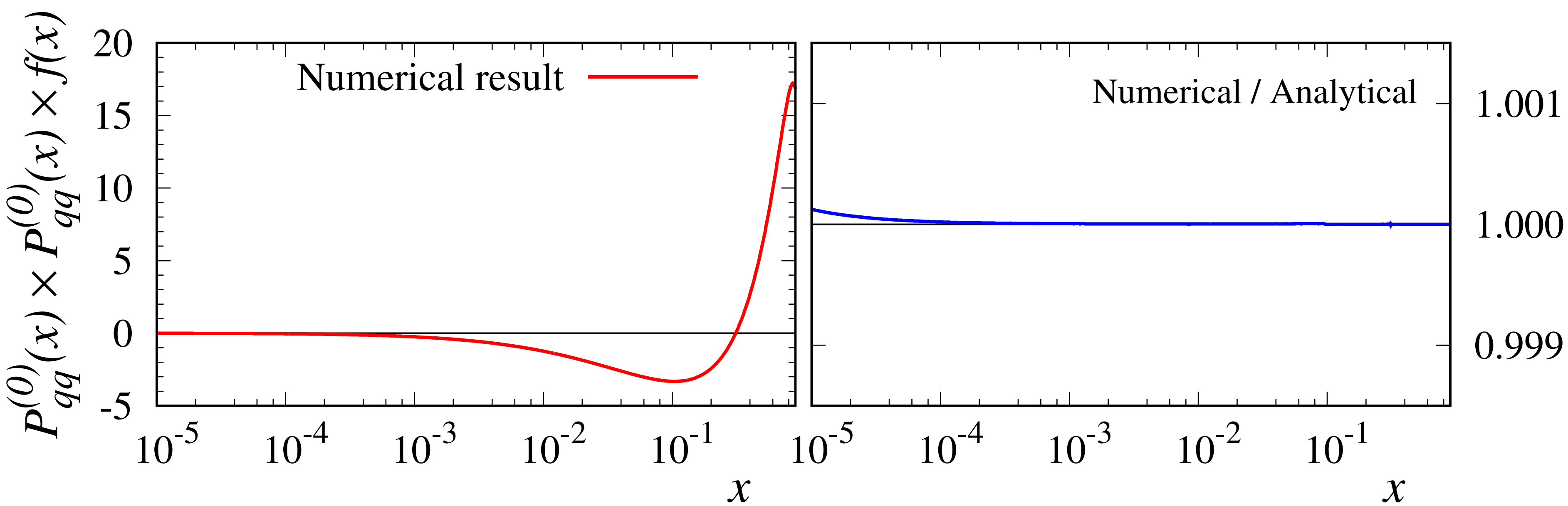
- An operation that is often needed is the convolution between operators:
  - involved in the computation of factorisation **scale variations**,
  - computation of the **PDF evolution operator**.

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

- Consider for example:

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

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



Evolution operator

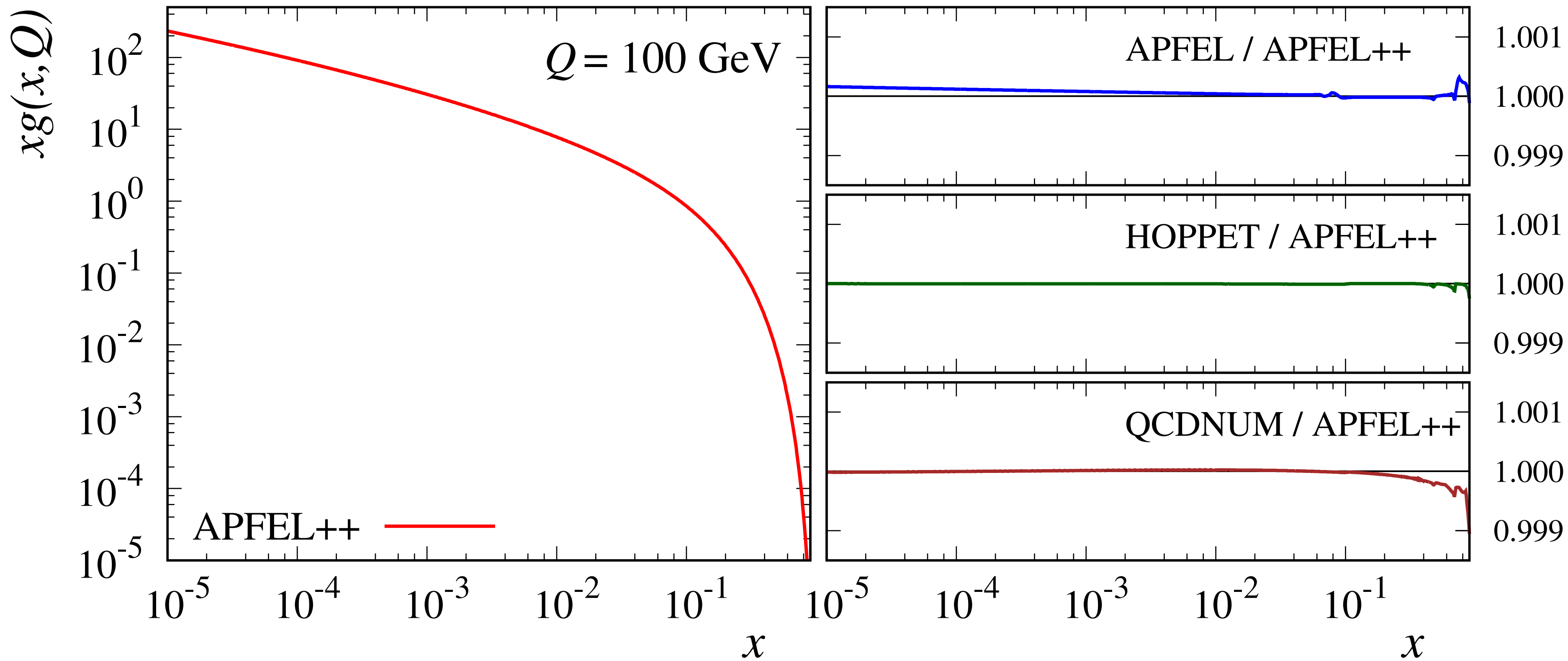
- The DGLAP can be written in terms the **evolution operator**:

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

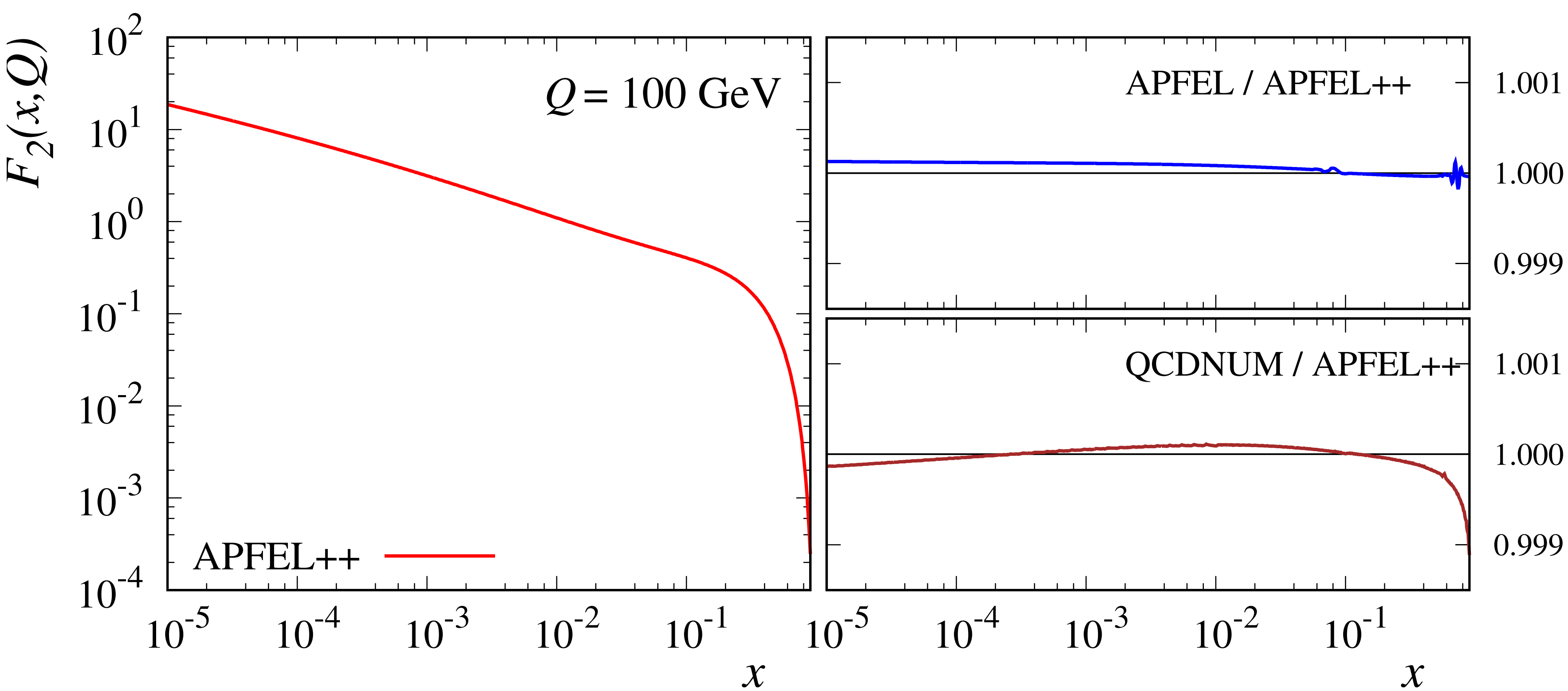
- The evolution operator can be used to evolve any initial scale PDF:
  - **harder** to compute than evolving PDFs directly,
  - it has to be computed **only once** (for each μ_0 and μ).
- This object is used for the construction of the **APFELgrid** tables:
  - extremely hard to compute in APFEL (Fortran),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

APFEL through LHAPDF

- Idea: delegate LHAPDF to interpolate over the (x, Q^2) grid:
  - more performing,
  - standardise the access to PDFs.

```cpp
// APFEL++ default EvolutionSetup object
apfel::EvolutionSetup es{};

// Feed it to the initialisation class of APFEL++
apfel::InitialiseEvolution ev{es, true};

// Construct pointer to LHAPDF::PDF object
LHAPDF::PDF* distAP = mkPDF(ev);

// Call PDFs
const std::map<int, double> PDFmap = distAP->xfxQ(x, mu);
```

APFEL++ evolution:
AlphaQCD(Q) = 1.1638e-01

x	u-ubar	d-dbar	2(ubr+dbr)	c+cbar	gluon
1.0e-05	5.0597e-03	2.9000e-03	2.9868e+01	1.3409e+01	1.8825e+02
1.0e-04	2.0510e-02	1.1486e-02	1.4191e+01	6.0136e+00	8.0275e+01
1.0e-03	7.7062e-02	4.3014e-02	6.0966e+00	2.3549e+00	2.9215e+01
1.0e-02	2.4305e-01	1.3669e-01	2.2041e+00	7.1400e-01	7.9998e+00
1.0e-01	5.1440e-01	2.4974e-01	3.9254e-01	7.5071e-02	8.9562e-01
3.0e-01	3.3154e-01	1.1785e-01	3.5867e-02	6.7898e-03	9.6761e-02
5.0e-01	1.0288e-01	2.6959e-02	2.4053e-03	5.4369e-04	9.5518e-03
7.0e-01	1.4110e-02	2.6031e-03	5.1163e-05	1.3984e-05	3.6137e-04
9.0e-01	1.8836e-04	2.4841e-05	2.1042e-08	8.2414e-09	7.3548e-07

LHAPDF (tabulated) evolution:
AlphaQCD(Q) = 1.1638e-01

x	u-ubar	d-dbar	2(ubr+dbr)	c+cbar	gluon
1.0e-05	5.0549e-03	2.9037e-03	2.9871e+01	1.3411e+01	1.8827e+02
1.0e-04	2.0510e-02	1.1491e-02	1.4193e+01	6.0140e+00	8.0282e+01
1.0e-03	7.7066e-02	4.3017e-02	6.0971e+00	2.3550e+00	2.9217e+01
1.0e-02	2.4306e-01	1.3670e-01	2.2043e+00	7.1472e-01	8.0004e+00
1.0e-01	5.1438e-01	2.4974e-01	3.9226e-01	7.5312e-02	8.9450e-01
3.0e-01	3.3153e-01	1.1785e-01	3.5865e-02	6.8228e-03	9.6755e-02
5.0e-01	1.0288e-01	2.6957e-02	2.4027e-03	5.4586e-04	9.5468e-03
7.0e-01	1.4109e-02	2.6030e-03	5.1163e-05	1.4071e-05	3.6138e-04
9.0e-01	1.8834e-04	2.4838e-05	2.1027e-08	8.3325e-09	7.3525e-07

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,
  - $\overline{\rm MS}$ 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 FORTRAN 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

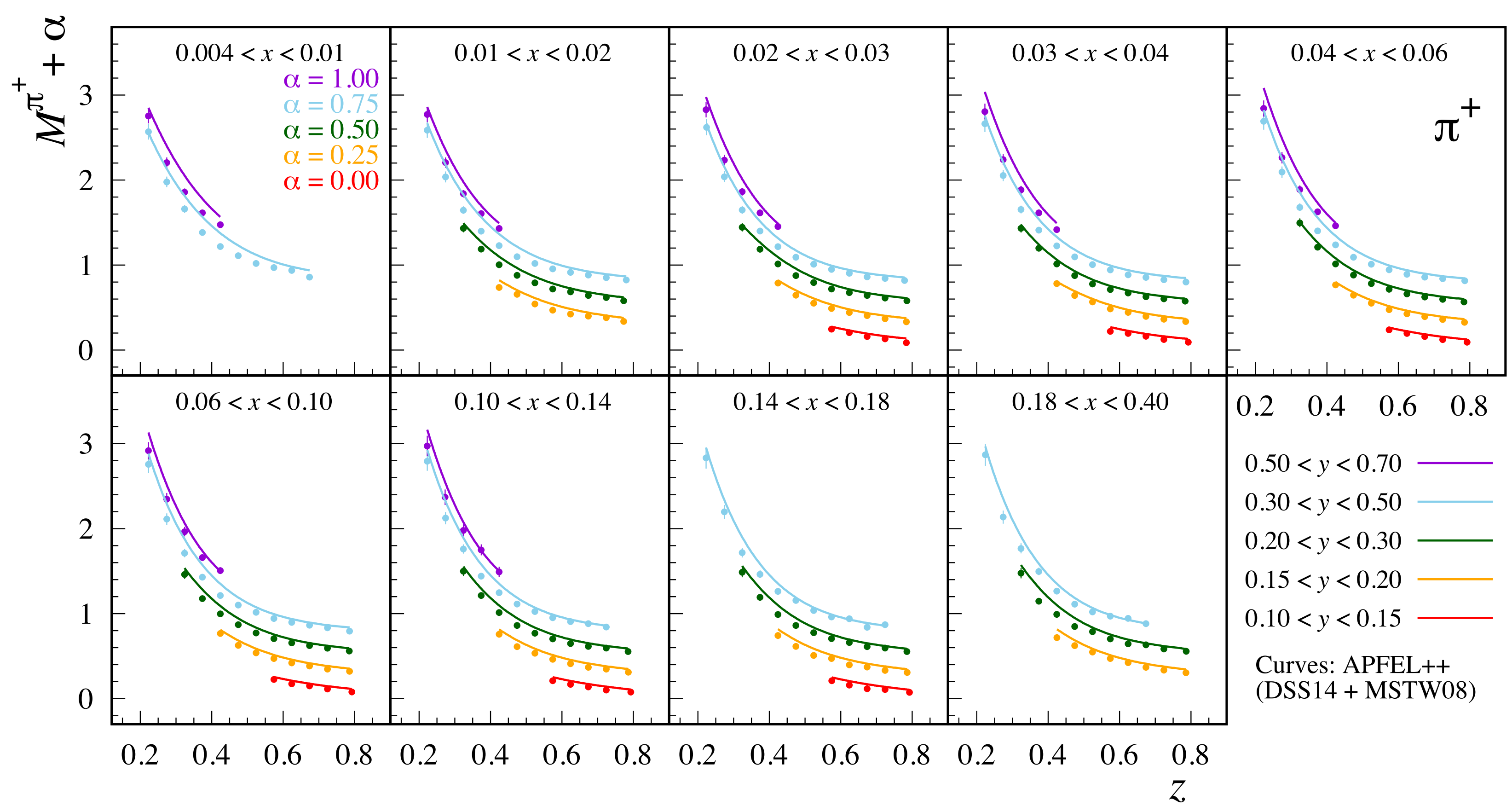
- SIDIS cross sections (integrated over q_T) have this structure:

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

- 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)

$$F_{f/P}(x, \mathbf{b}_T; \mu, \zeta) = \sum_j C_{f/j}(x, b_*; \mu_b, \zeta_F) \otimes f_{j/P}(x, \mu_b) \quad : A$$

$$\times \exp\left\{ K(b_*; \mu_b) \ln \frac{\sqrt{\zeta_F}}{\mu_b} + \int_{\mu_b}^{\mu} \frac{d\mu'}{\mu'} \left[\gamma_F - \gamma_K \ln \frac{\sqrt{\zeta_F}}{\mu'} \right] \right\} \quad : B$$

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

TMD Evolution (PDFs)

$$F_{f/P}(x, \mathbf{b}_T; \mu, \zeta) = \sum_j C_{f/j}(x, b_*; \mu_b, \zeta_F) \otimes f_{j/P}(x, \mu_b) \quad : A$$

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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

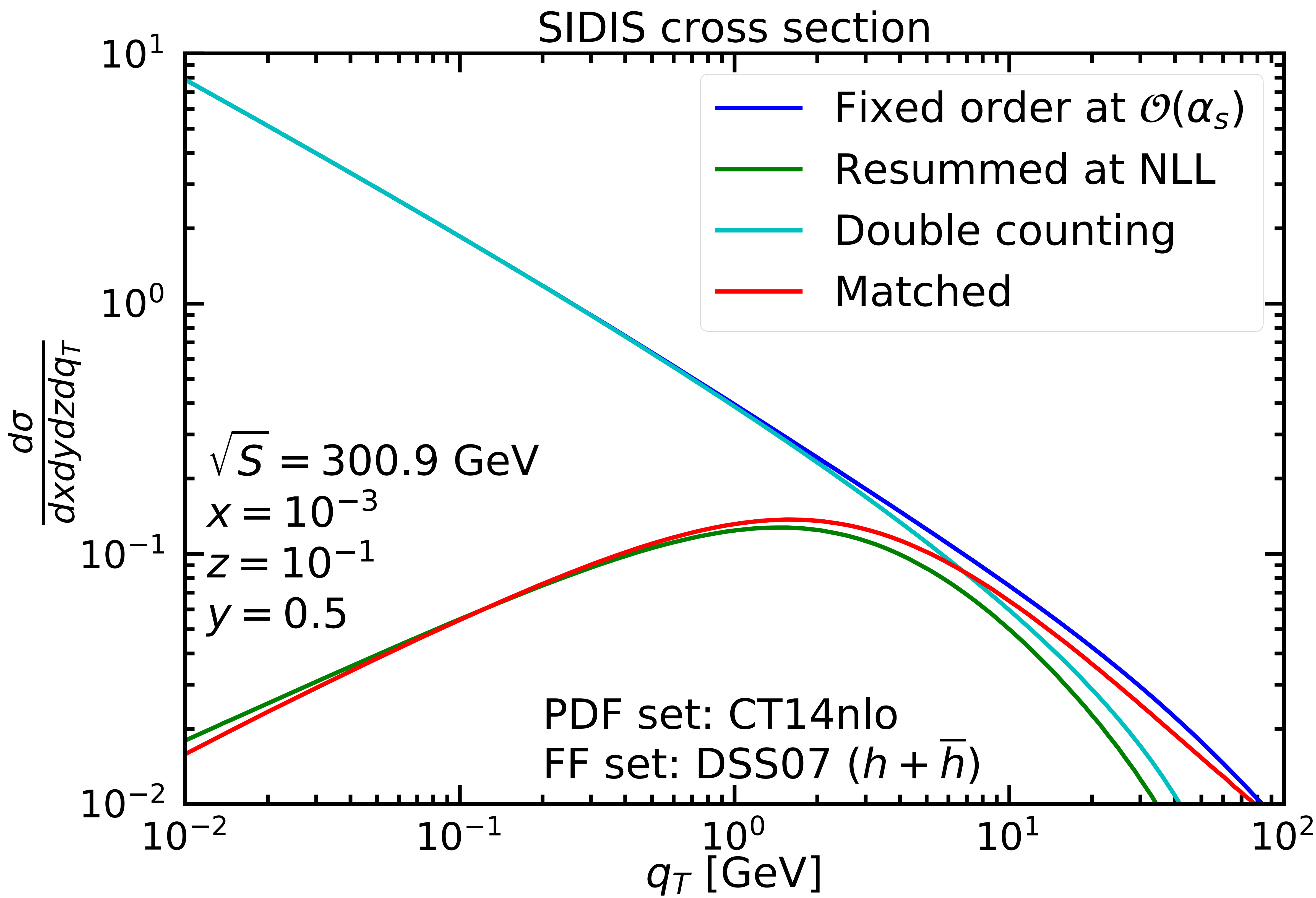
- In SIDIS, what enters the computation of the cross sections is:

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

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

- 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).