The new theory prediction ~~pipeline~~ pineline and towards N3LO PDF

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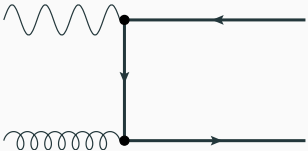
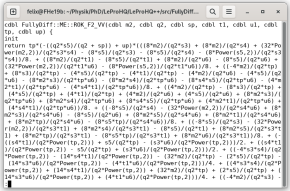
Outline

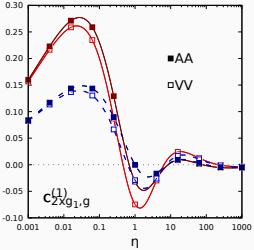
1. The new theory `pineline`

[2302.12124]

1.1. Motivation

Including New Computations

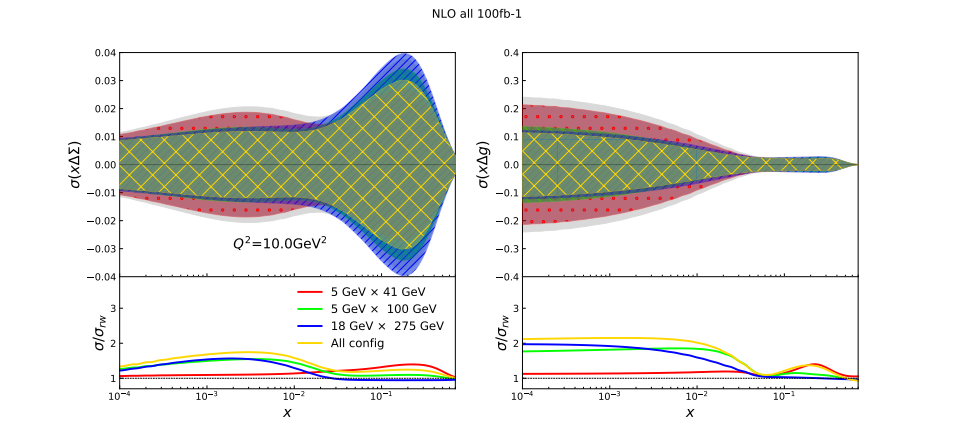
- Computing new observables is expensive both in runtime (days/weeks) and development time (month/years)
- E.g. NLO heavy quark production in polarized DIS [PRD98.014018] [1910.01536] [PRD104.016033]
-  → 

→ 

- How to measure the actual impact on PDFs?

Reweighting

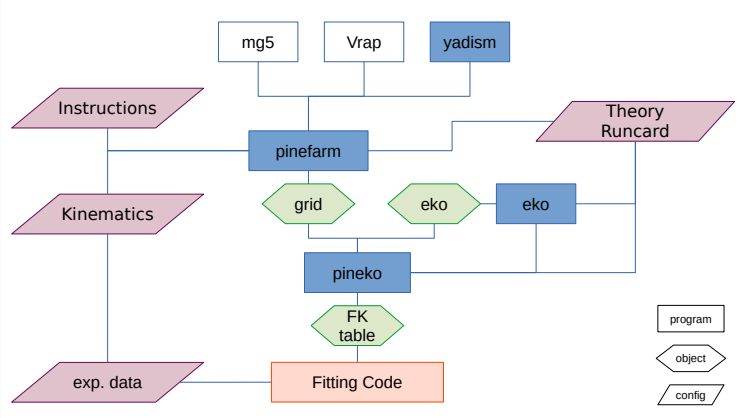
Reweighting is possible [PRD104.114039] - and even needed for the EIC



but a new PDF fit would be better!

New Theory Prediction Pipeline

Produce FastKernel (FK) tables!



The workhorse in the background: PineAPPL

New Theory Prediction Pipeline

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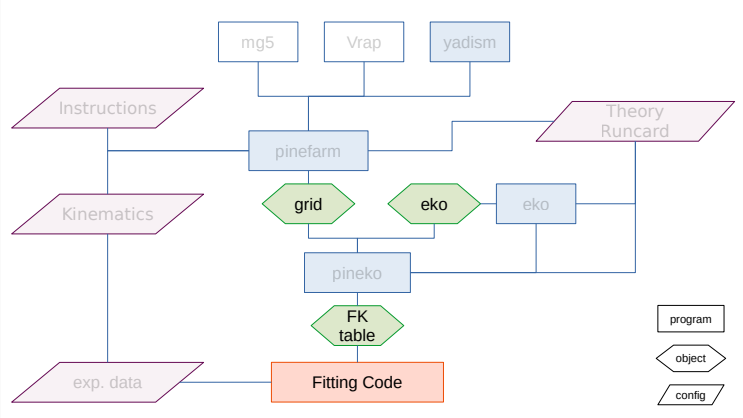

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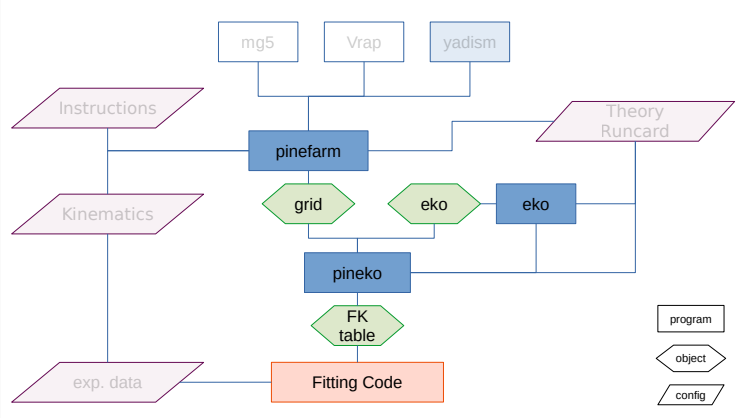

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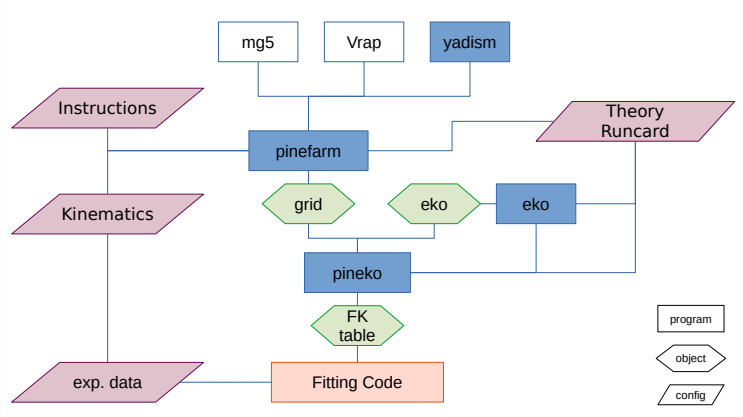
New Theory Prediction Pipeline

Produce FastKernel (FK) tables!



The workhorse in the background: PineAPPL

`pineline`: Industrialization of High-Energy Theory Predictions [2302.12124]

`https://nnpdf.github.io/pineline`

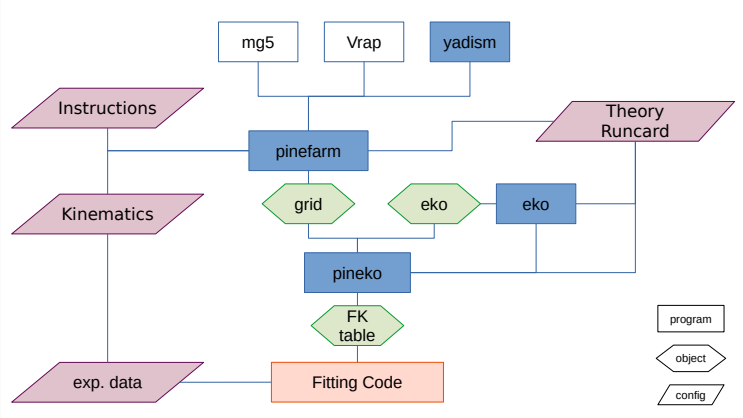
- **Industrialization**: collect diverse generators in an "assembly line"
  $\rightarrow$ NNPDF4.0[EPJC82.428]: $>$ 4.5k datapoints $+$ $>$ 10 generators
- **I/O format**: single input $\rightarrow$ translation layer $\rightarrow$ single output
- **Reproducibility**: track data and metadata
- **Open Source**: crucial to the above

$\Rightarrow$ please provide new calculations in an "interfaceable" way

1.2. PineAPPL [JHEP12.108]

New Theory Prediction Pipeline

Produce FastKernel (FK) tables!



The workhorse in the background: PineAPPL

About PineAPPL

PineAPPL is a fast interpolation grid library that

- extends to arbitrary orders in QCD and EW coupling
- provides a very good Command Line Interface
- provides several interfaces: C, C++, Fortran, Rust, Python
- can convert APPLgrid [EPJC66.503] and FastNLO [DIS12.217]

Check the documentation: `https://nnpdf.github.io/pineappl/`

The Command Line Interface (CLI)

The CLI (`pineappl`) serves for the everyday life questions:

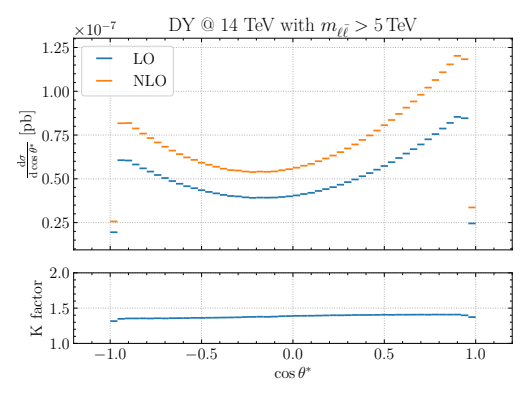
- `convolute` - get the predictions for any PDF set including uncertainties
- `channels` - split the predictions into luminosity channels
- `orders` - split the predictions into perturbative orders
- `info` - access meta data
- `plot` - generate a (customizable) python plot script

The Command Line Interface

```
$ pineappl convolute CMS_DY_14TEV_MLL_5000_COSTH.pineappl.lz4 \
     NNPDF40_nnlo_as_01180
b        costh     dsig/dcosth  scale uncertainty
          []           [pb]            [%]
--+-------+------+------------+--------+--------
0       -1   -0.96 5.0382145e-8    -4.73     4.32
1   -0.96   -0.92 1.6366674e-7    -4.98     4.62
2   -0.92   -0.88 1.6611145e-7    -5.06     4.70
3   -0.88   -0.84 1.5983761e-7    -5.08     4.74
4   -0.84    -0.8 1.5374426e-7    -5.09     4.75
5    -0.8   -0.76 1.4800320e-7    -5.10     4.76
6   -0.76   -0.72 1.4238050e-7    -5.10     4.76
7   -0.72   -0.68 1.3708378e-7    -5.10     4.76
8   -0.68   -0.64 1.3191722e-7    -5.12     4.78
[...]
```

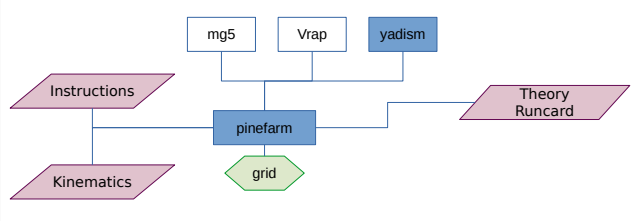
The Python Interface

```python
import lhapdf
import pineappl
# load PDF
pdf = lhapdf.mkPDF("NNPDF40_nnlo_as_01180",0)
# load grid
grid = pineappl.grid.Grid.read("CMS_DY_14TEV_MLL_5000_COSTH.pineappl.lz4")
# convolute
print(grid.convolute_with_one(2212,pdf.xfxQ2,pdf.alphasQ2))
# prints the same list of numbers
```



1.3. `pinefarm`

Interface to Other Programs: `pinefarm`




```
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*                    *                   *                      *
*                      * * * *   5   * * * *                    *
*                    *                   *                      *
*                  *                       *                    *
*                                                               *
*    The MadGraph5_aMC@NLO Development Team - Find us at        *
*    https://server06.fynu.ucl.ac.be/projects/madgraph          *
*                                and                            *
*                  http://amcatnlo.cern.ch                      *
*                                                               *
*                     Code download from:                       *
*              https://launchpad.net/madgraph5                  *
*                                                               *
*    Please refer to: MadGraph5_aMC@NLO paper                   *
*                 J. Alwall et al.                              *
*                 arXiv:1405.0301, JHEP 1407 (2014) 079         *
*****************************************************************
```

[in preparation]

Vrap [PRD69.094008]

more MC interfaces coming soon (e.g. MATRIX [EPJC78.537])

A Monte Carlo Example using C++

For a more complete example see: examples directory in PineAPPL repo

```cpp
void fill_grid(PineAPPL::Grid &grid, std::size_t calls) {
    // MC loop
    for (std::size_t i = 0; i != calls; ++i) {
        // generate a phase-space point
        auto tmp = hadronic_pspgen(rng, 10.0, 7000.0);
        // compute kinematics
        double ptl = sqrt((t * u / s));
        // apply cuts
        if (ptl < 14.0) continue;
        // fill grid - here binning in |y_ll|
        auto weight = jacobian * matrix_element(s, t, u);
        grid.fill(x1, x2, q2, 0, fabs(yll), 0, weight);
    }
}
```

The `pinecards` repo

Collect available observables: `https://github.com/NNPDF/pinecards`

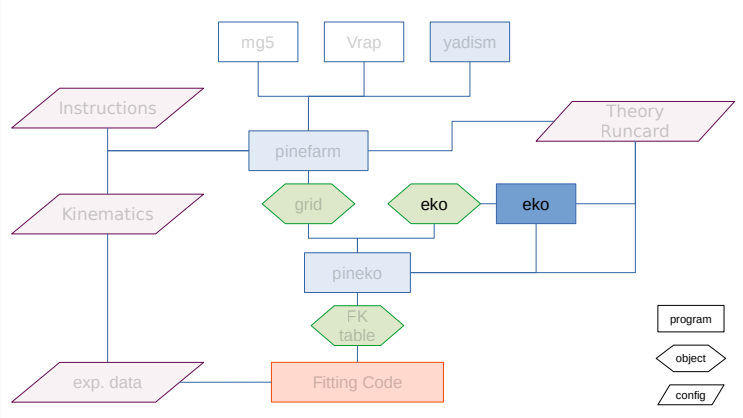
ATLAS_TTB_8TEV_LJ_TTRAP	Fix ordering of model loading and model-specific settings	2 weeks ago
ATLAS_TTB_8TEV_TOT	Fix ordering of model loading and model-specific settings	2 weeks ago
ATLAS_WM_7TEV	Fix ordering of model loading and model-specific settings	2 weeks ago
ATLAS_WP_7TEV	Fix ordering of model loading and model-specific settings	2 weeks ago
BCDMS_NC_EM_D_F2	Export pinefarm to its own repo	3 months ago
BCDMS_NC_EM_P_F2	Export pinefarm to its own repo	3 months ago
CHORUS_CC_NB_PB_SIGMARED	Export pinefarm to its own repo	3 months ago
CHORUS_CC_NU_PB_SIGMARED	Export pinefarm to its own repo	3 months ago
CMS_2JET_7TEV_0005	Fix ordering of model loading and model-specific settings	2 weeks ago
CMS_2JET_7TEV_0510	Fix ordering of model loading and model-specific settings	2 weeks ago
CMS_2JET_7TEV_1015	Fix ordering of model loading and model-specific settings	2 weeks ago

a similar effort for the experimental data is ongoing!

1.4. EKO [EPJC82.976]

New Theory Prediction Pipeline

Produce FastKernel (FK) tables!



The workhorse in the background: PineAPPL

EKO Definition

EKO

Evolution Kernel Operators

DGLAP:

$$\mu_F^2 \frac{\mathrm{d}\mathbf{f}}{\mathrm{d}\mu_F^2}(\mu_F^2) = \mathbf{P}(a_s(\mu_R^2), \mu_F^2) \otimes \mathbf{f}(\mu_F^2)$$

as operator equation for the evolution kernel operator (EKO) $\mathbf{E}$:

$$\mu_F^2 \frac{\mathrm{d}}{\mathrm{d}\mu_F^2}\mathbf{E}(\mu_F^2 \leftarrow \mu_{F,0}^2) = \mathbf{P}(a_s(\mu_R^2), \mu_F^2) \otimes \mathbf{E}(\mu_F^2 \leftarrow \mu_{F,0}^2)$$

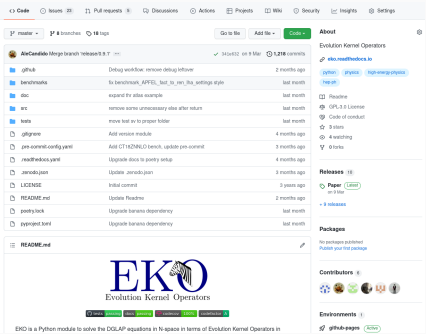
with

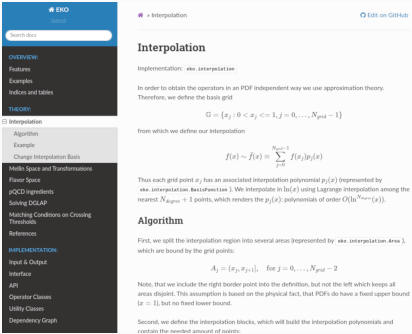
$$\mathbf{f}(\mu_F^2) = \mathbf{E}(\mu_F^2 \leftarrow \mu_{F,0}^2) \otimes \mathbf{f}(\mu_{F,0}^2)$$

EKO Physics Features

- independent of boundary condition $\rightarrow$ PDF fitting
- Mellin (N-) space solution, but momentum (x-) space delivery via piecewise Lagrange-interpolation
- Intrinsic heavy quark distributions
- Backward VFNS evolution (i.e. across thresholds and with intrinsic)

EKO Project Management

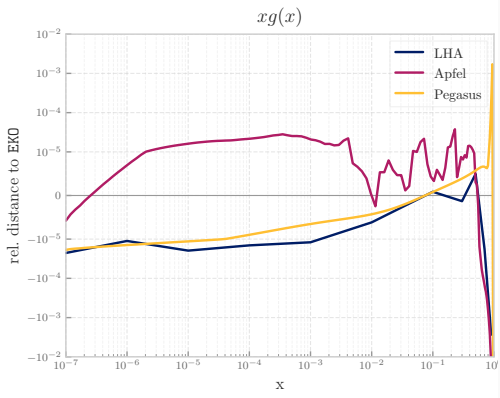


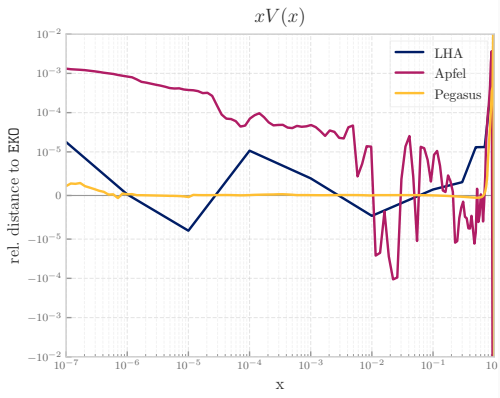


- Fully open source: `https://github.com/NNPDF/eko`
- Written in Python
- Fully documented: `https://eko.readthedocs.io/`

EKO Benchmarks

LHA benchmark [0204316][0511119]:

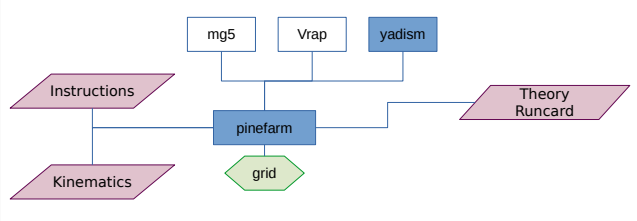




$\Rightarrow$ EKO is working!

1.5. `yadism` [in preparation]

Interface to Other Programs: `pinefarm`




```
*****************************************************************
*                                                               *
*   W E L C O M E  t o  M A D G R A P H 5 _ a M C @ N L O       *
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*                      * * * *  5  * * * *                      *
*                    *                   *                      *
*                  *                       *                    *
*                                                               *
*                                                               *
*    The MadGraph5_aMC@NLO Development Team - Find us at        *
*    https://server06.fynu.ucl.ac.be/projects/madgraph          *
*                                and                            *
*                 http://amcatnlo.cern.ch                       *
*                                                               *
*                    Code download from:                        *
*              https://launchpad.net/madgraph5                  *
*                                                               *
*    Please refer to: MadGraph5_aMC@NLO paper                   *
*                 J. Alwall et al.                              *
*                 arXiv:1405.0301, JHEP 1407 (2014) 079         *
*****************************************************************
```

[in preparation]

Vrap [PRD69.094008]

more MC interfaces coming soon (e.g. MATRIX [EPJC78.537])

yadism Physics Features

- DIS coefficient function database
- independent of boundary condition → PDF fitting
- separate features: TMC, FNS
- constant benchmark against APFEL

same improvement in terms of project management as EKO!

https://github.com/NNPDF/yadism

https://yadism.readthedocs.io

Coefficient Functions

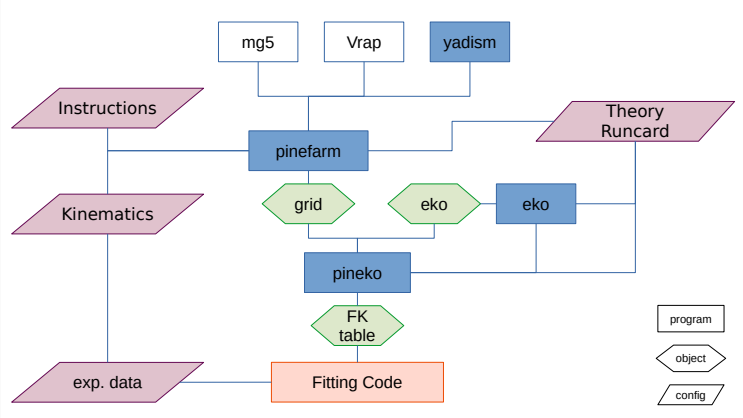
- implemented coefficient functions:

	light	heavy	intrinsic
NC	$O(a_s^2)$ [VVM05,MVV05,MV00]	$O(a_s^2)$ [Hek19]	$O(a_s)$ [KS98]
CC	$O(a_s^2)$ [MRV08,MVV09]	$O(a_s)$ [GKR96]	$O(a_s)$ [in prep.]

- implemented flavor number schemes: FFNS, ZM-VFNS, FONLL

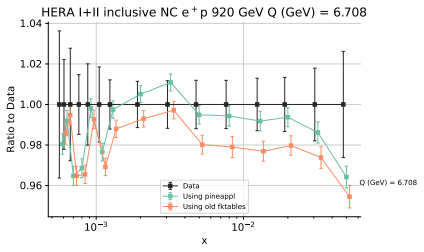
New Theory Prediction Pipeline

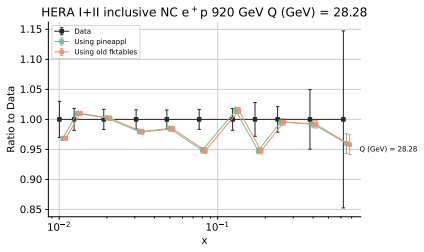
Produce FastKernel (FK) tables!

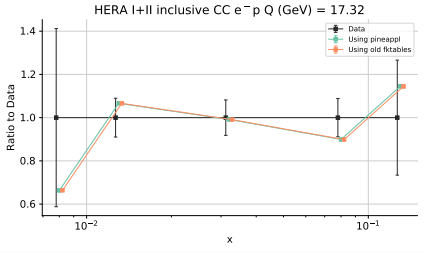


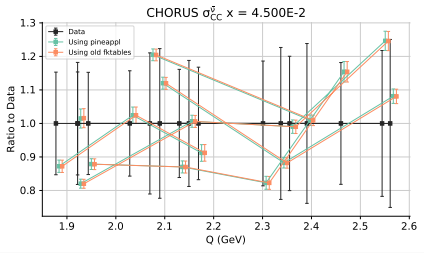
The workhorse in the background: PineAPPL

Comparison `yadism` against `APFEL`









green, "pineappl" = `pineline` vs. orange, "old" = `APFEL`

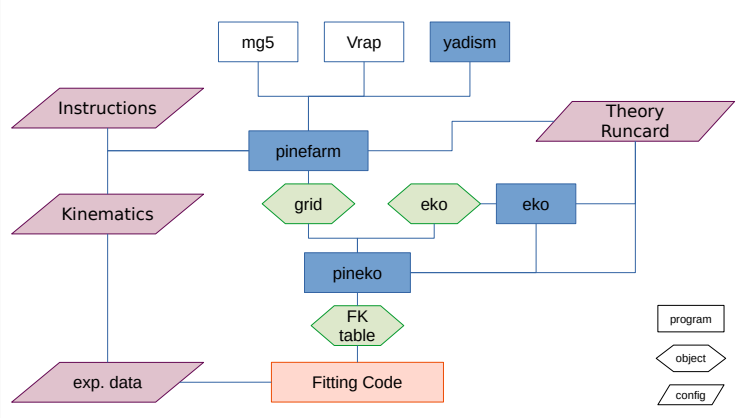
1.6. Outlook

Outlook

- extend to N3LO $\rightarrow$ see part 2
- include missing higher order uncertainty (MHOU)
- include QED corrections
- add polarized setup
- extend to fragmentation function
- add EW corrections
- ...

New Theory Prediction Pipeline

Produce FastKernel (FK) tables!



The workhorse in the background: PineAPPL

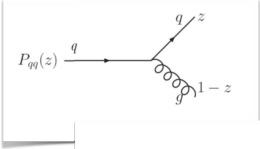
2. Towards N3LO PDFs [in preparation]

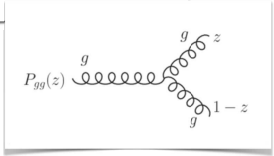
Roadmap towards N3LO PDFs

- DGLAP @ N3LO $\rightarrow$ splitting functions approximation ✓
- DIS @ N3LO $\rightarrow$ light + massive coefficient functions
- LHC observables @ NNLO + K-factors
- Inclusion of theory uncertainties both from scale variations and N3LO accuracy

N3LO singlet sector

Analytical calculations of the complete N3LO spitting functions are not available yet. Restricting to the singlet sector the known limits are:





large-n_f

- Davies, Vogt, Ruijl, Ueda, and Vermaseren. Large-n_f contributions to the four-loop splitting functions in QCD. [arXiv:1610.07477]

small-x

- Bonvini and Marzani. Four-loop splitting functions at small-x. [arXiv:1805.06460]
- Davies, Kom, Moch, and Vogt. Resummation of small-x double logarithms in QCD: inclusive deep-inelastic scattering. 2 2022. arXiv:2202.10362.

large-x

- Duhr, Mistlberger, and Vita. Soft integrals and soft anomalous dimensions at N3LO and beyond. [arXiv:2205.04493].
- Henn, Korchemsky, and Mistlberger. The full four-loop cusp anomalous dimension in $\mathcal{N} = 4$ super Yang-Mills and QCD. [arXiv:1911.10174].
- Soar, Moch, Vermaseren, and Vogt. On Higgs–exchange DIS, physical evolution kernels and fourth-order splitting functions at large x. [arXiv:0912.0369].

Moments

- Moch, Ruijl, Ueda, Vermaseren, and Vogt. Low moments of the four-loop splitting functions in QCD. [arXiv:2111.15561]. $+2302.07593$

- Theoretical inputs are not enough to determine the full expressions analytically.
- Need to parametrise the unknown part with sub-leading contributions.
- Uncertainties from this determination has to be taken into account during the fit.

Singlet

	n_f^0	n_f^1	n_f^2	n_f^3
$\gamma_{gg}^{(3)}$	✓	✓	✓	✓
$\gamma_{gq}^{(3)}$	✓	✓	✓	✓
$\gamma_{qg}^{(3)}$		✓	✓	✓
$\gamma_{qq,ps}^{(3)}$		✓	✓	✓

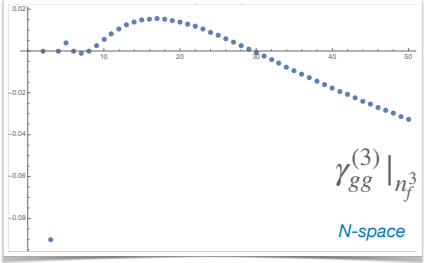
For results about the Non Singlet sector see backup

Approximation of $P_{gg}(x)$

$$\tilde{f}(N) = \int_0^1 x^{N-1} f(x) dx$$

Rule of thumb:
small-N → small-x,
large-N → large-x

Comparison w.r.t. known analytical part (%)



The approximation procedure is performed in Mellin space for each n_f part independently:

1. Parametrise the difference between the *4* known moments and known limits with *4* functions $f_i(N)$.

2. Varying the sub-leading unknown $f_i(N)$ to produce a large set of parameterisation candidates (≈ 70).

3. Reduce the number of samples discarding too wiggly parameterisations and looking at the most representative cases.

In $P_{gg}(x)$:

Theoretical constrain include:

- large-N:

$$\gamma_{gg}^{(3)}(N \to \infty) \approx \Gamma_A S_1(N) + B_{gg} + \mathcal{O}(\frac{\ln(N)}{N})$$

- small-N pole at $N = 0$, and $N = 1$ *(leading contribution)*:

$$\gamma_{gg}^{(3)}(N \to 1) \approx C_4 \frac{1}{(N-1)^4} + C_3 \frac{1}{(N-1)^3} + \mathcal{O}((N-1)^{-2})$$

- 4 lowest moments $N = \{2,4,6,8\}$

Solve the constrain given by the 4 known Mellin moments with many different candidates $\{f_1, f_2, f_3, f_4\}$:

$$f_1 = \frac{S_1(N)}{N}, \; f_2 = \frac{1}{(N-1)^2}$$

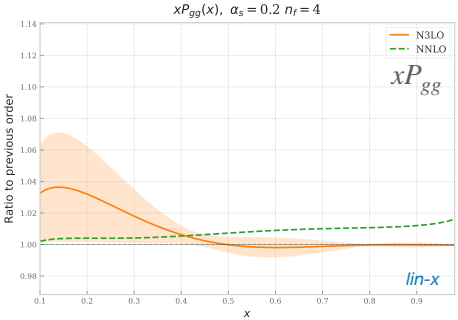
$$f_3 = \{ \frac{1}{(N-1)}, \frac{1}{N} \}$$

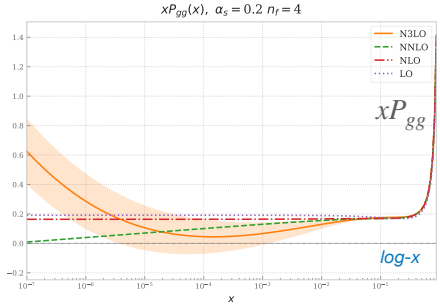
$$f_4 = \{ \frac{1}{(N-1)}, \frac{1}{N^4}, \frac{1}{N^3}, \frac{1}{N^2}, \frac{1}{N}, \frac{1}{(N+1)^3}, \frac{1}{(N+1)^2},$$

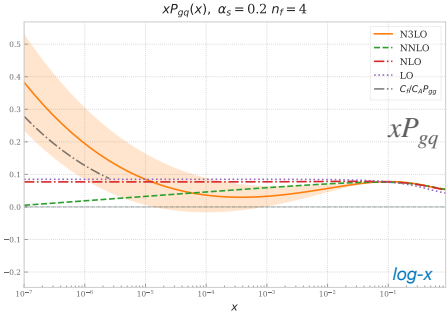
$$\frac{1}{N+1}, \frac{1}{N+2}, \mathscr{M}[\ln(1-x)], \mathscr{M}[(1-x)\ln(1-x)], \frac{S_1(N)}{N^2} \}$$

N3LO singlet sector

PRELIMINARY RESULTS



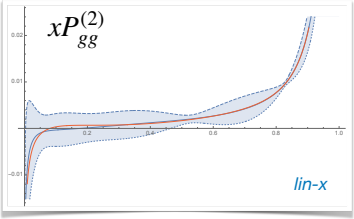


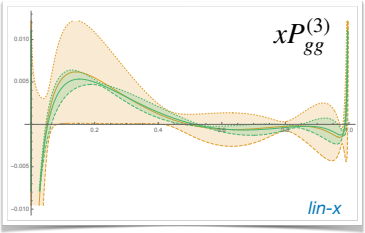


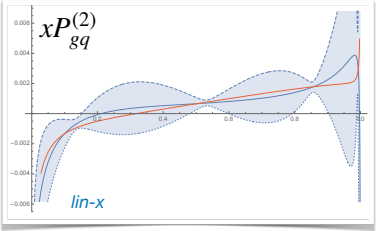
- Singlet approximated spitting functions are less constrained by the known limits. The coefficients of $1/x\ln^2(x)$, $1/x\ln(x)$ play a crucial role in the small-x region.
- Uncertainty arising from the approximation is not negligible.
- Off diagonal terms P_{qg}, P_{gq} are more difficult to estimate (large-N goes to 0).
- Only theoretical inputs are considered.
- All the implemented approximations respect momentum sum rules.

Approximation checks

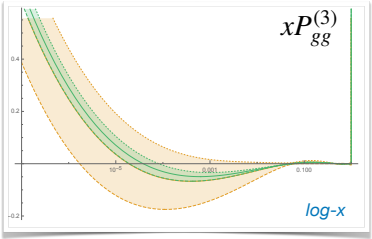
1. A possible way to validate the procedure is to **reproduce the known NNLO** singlet splitting functions using the very similar constrain that we have right now on the N3LO ones.



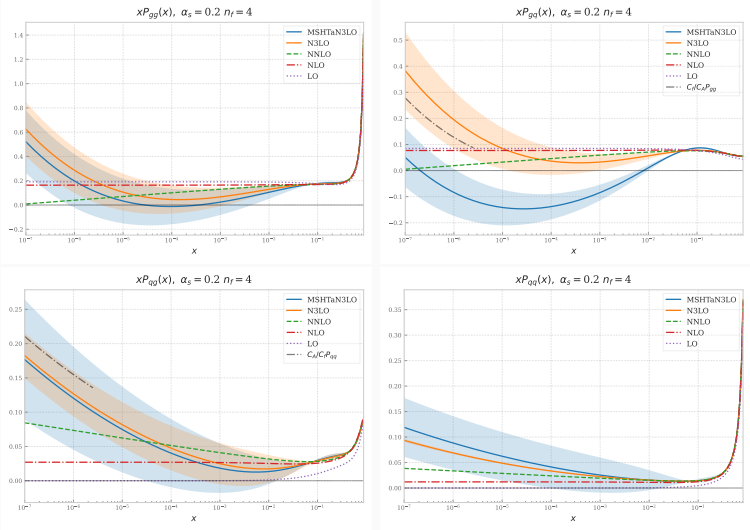




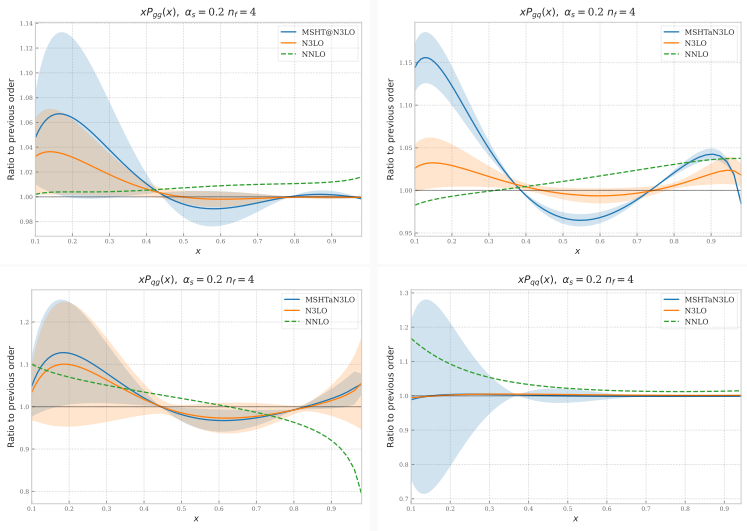
2. Another way to validate the results is to **interpolate the known moments**, and construct a more constrained parametrisation now including 5/6 moments.
If the procedure is working (the samples are varied enough) the uncertainty band obtained in this way should be small than the default one.



Comparison with MSHT [EPJC83.185] at small-x - PRELIMINARY!



Comparison with MSHT [EPJC83.185] at large-x - PRELIMINARY!



DIS @ N3LO

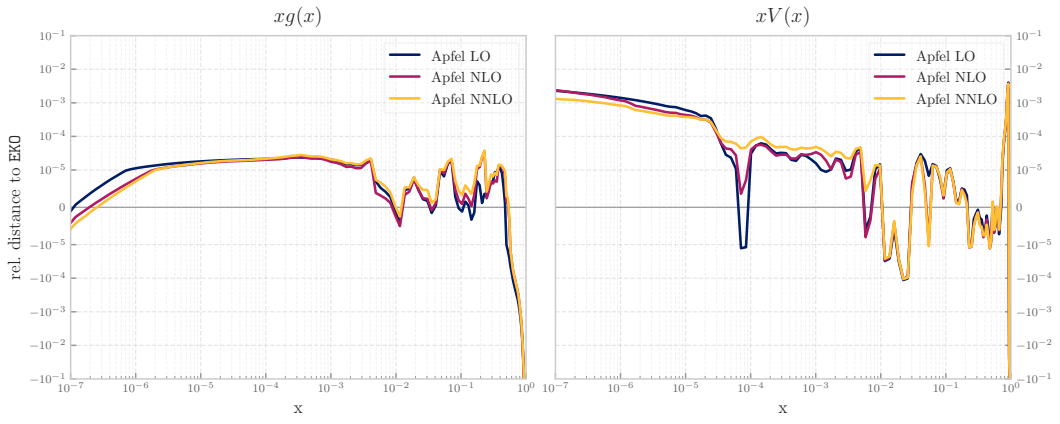
- light coefficient functions [VVM05],[MVV05],[MV00],[MRV08],[MVV09] ✓
- massive coefficient functions → approximation in MSc thesis of N. Laurenti ✓
- FONLL [FLNR10] prescription → MSc thesis of S. Zanioli, A. Barontini ✓
  or better: use "Numerical FONLL" (thanks to new `pineline`)

$$F^{\mathrm{FONLL}} = F^{(n_f+1)} + F^{(n_f)} - F^{(n_f,0)}$$

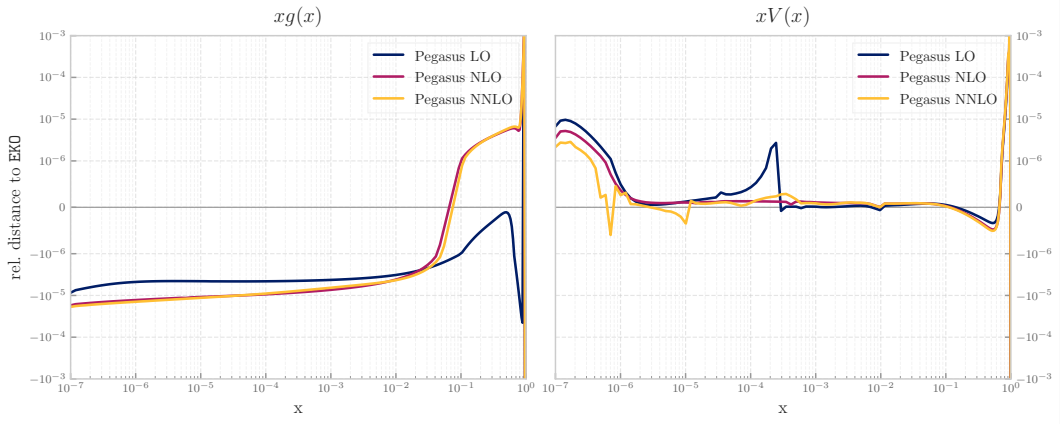
Thank you!

3. Backup slides

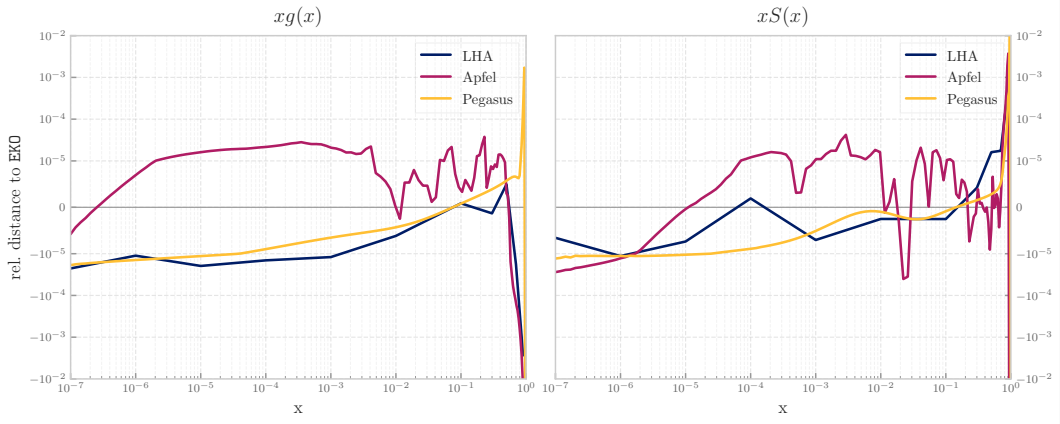
EKO APFEL benchmark



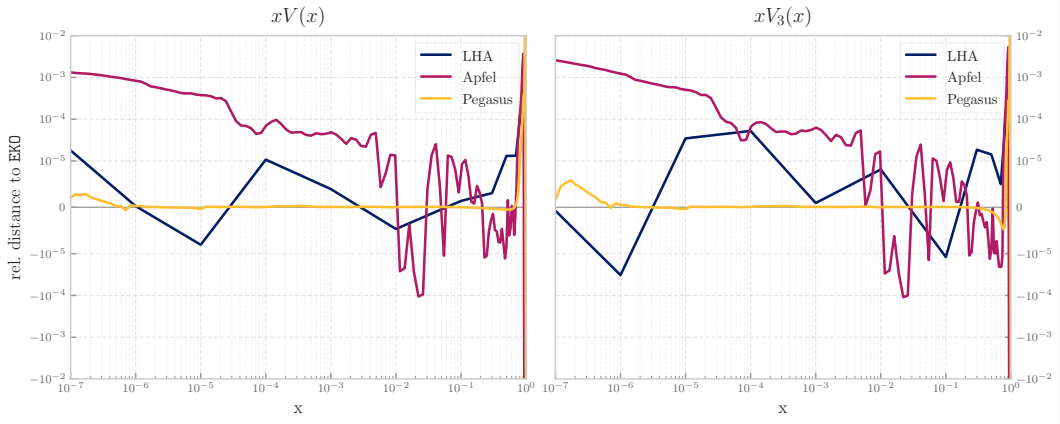
EKO PEGASUS benchmark



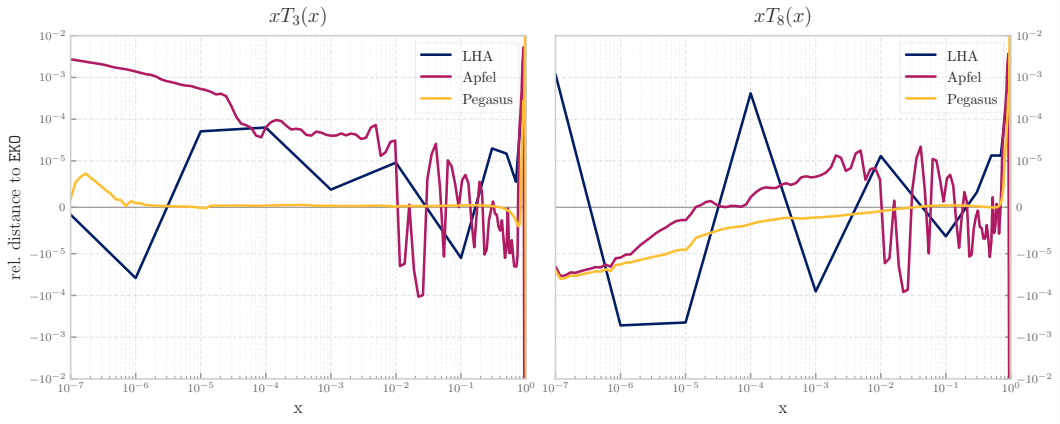
EKO LHA benchmark: g and Σ



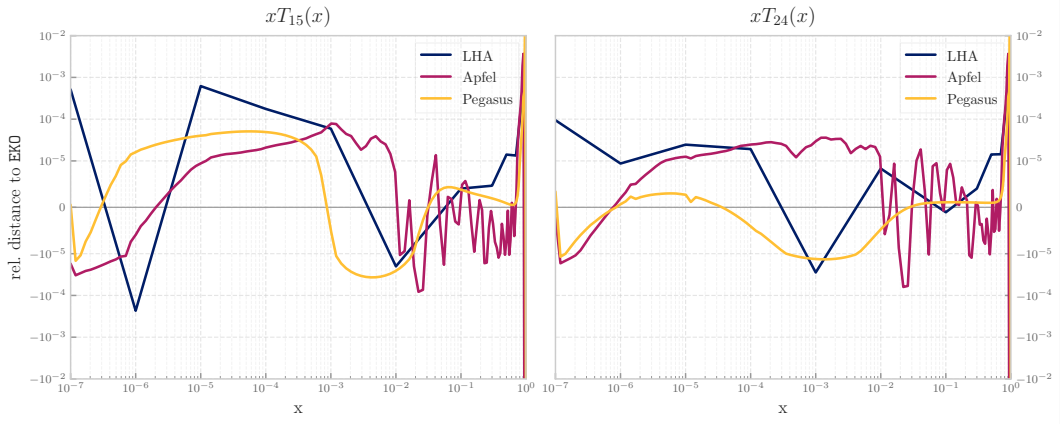
EKO LHA benchmark: V and V_3



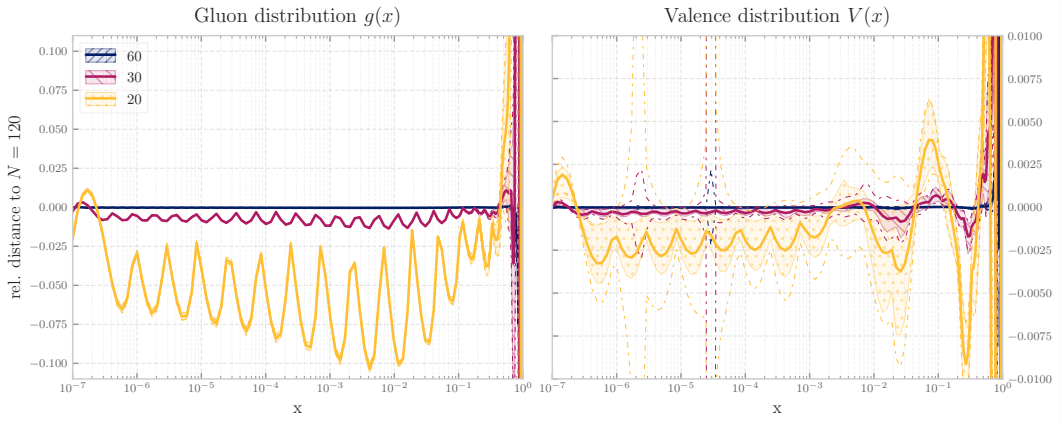
EKO LHA benchmark: T_3 and T_8



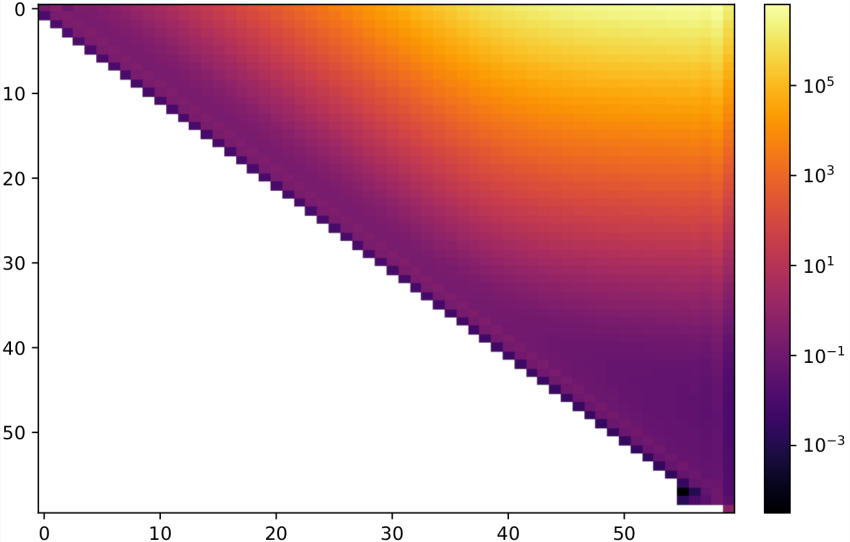
EKO LHA benchmark: T_{15} and T_{24}



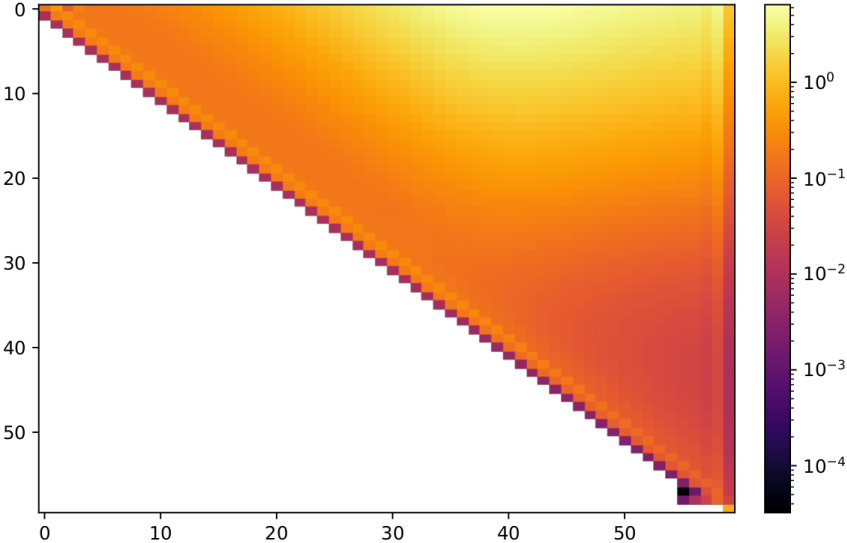
EKO Interpolation Error



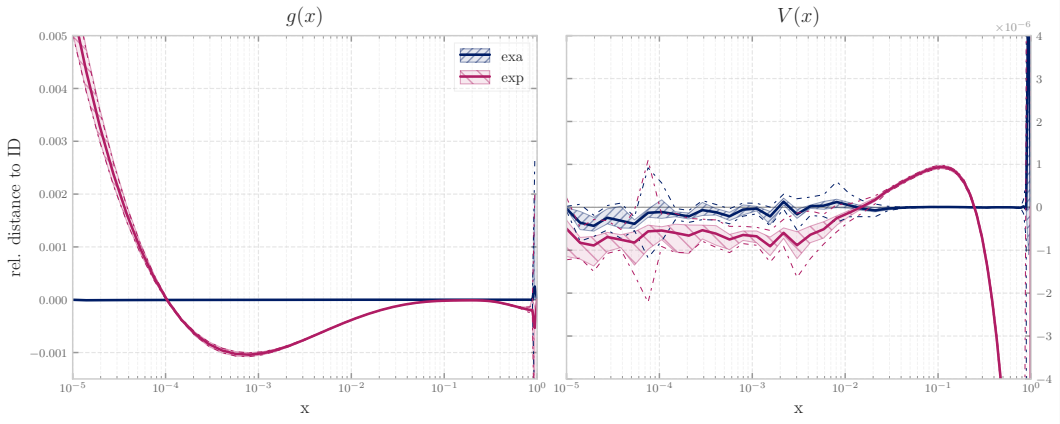
EKO Snapshot $S \leftarrow S$



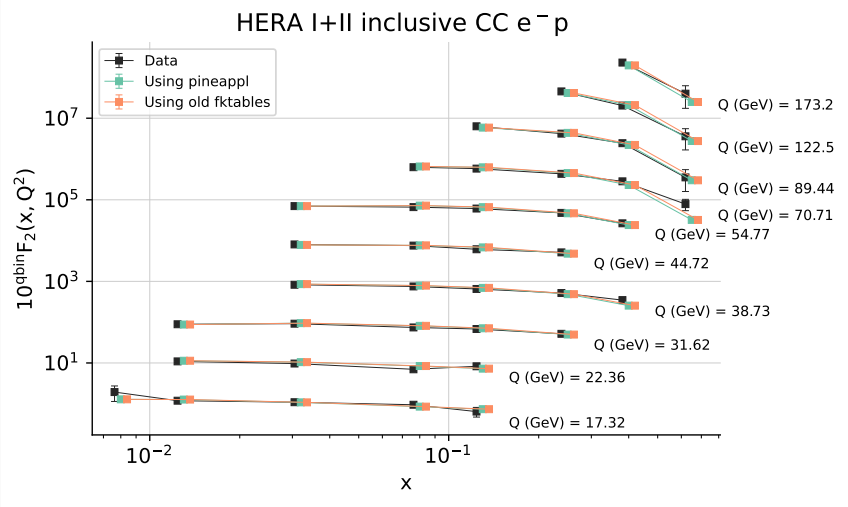
EKO Snapshot $V \leftarrow V$



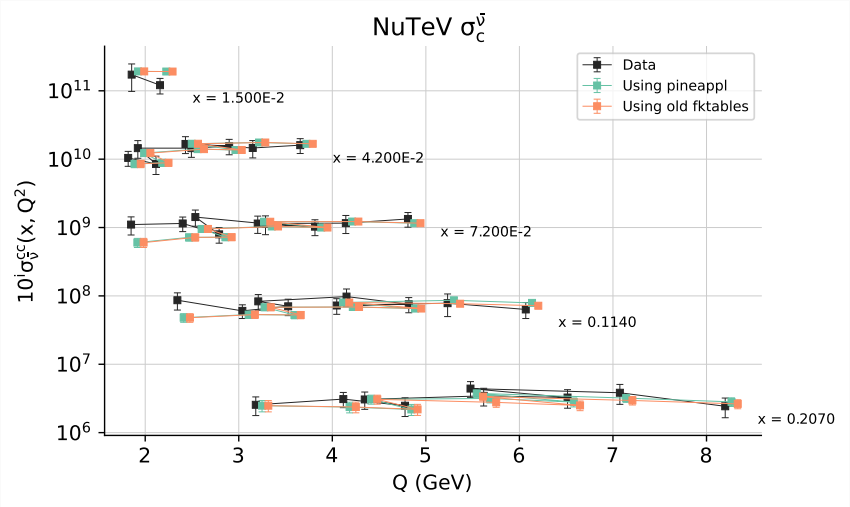
EKO Backward Evolution



Comparison `yadism` against `APFEL`

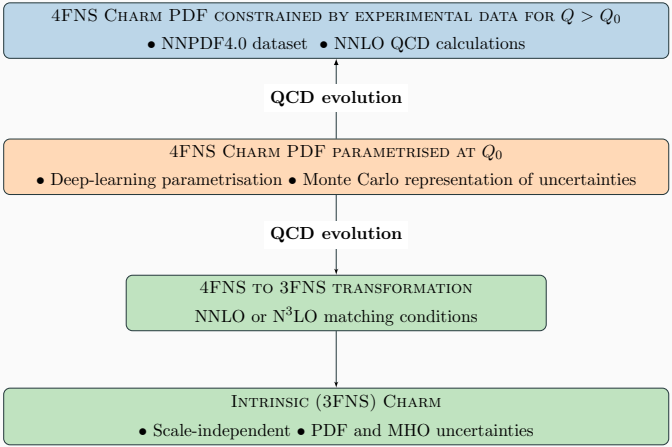


Comparison yadism against APFEL



Intrinsic Charm: Strategy

based on NNPDF4.0 [EPJC82.428]



Matching Conditions and Backward Evolution

For (forward) evolution across a matching scale μ_h^2:

$$\tilde{\mathbf{f}}^{(n_f+1)}(\mu_{F,1}^2) = \tilde{\mathbf{E}}^{(n_f+1)}(\mu_{F,1}^2 \leftarrow \mu_h^2)\mathbf{R}^{(n_f)}\tilde{\mathbf{A}}^{(n_f)}(\mu_h^2)\tilde{\mathbf{E}}^{(n_f)}(\mu_h^2 \leftarrow \mu_{F,0}^2)\tilde{\mathbf{f}}^{(n_f)}(\mu_{F,0}^2) \tag{1}$$

with $\mathbf{R}^{(n_f)}$ a flavor rotation matrix and $\tilde{\mathbf{A}}^{(n_f)}(\mu_h^2)$ the operator matrix elements (partially known up to N^{3}LO)

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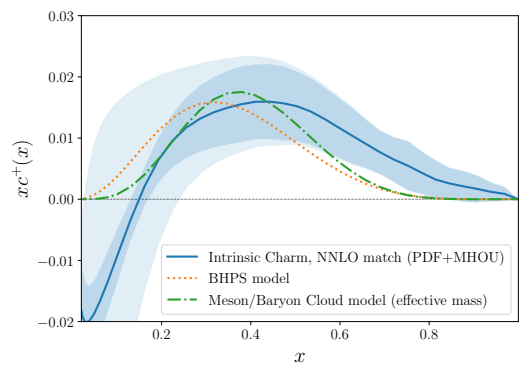
with $\mathbf{R}^{(n_f)}$ a flavor rotation matrix and $\tilde{\mathbf{A}}^{(n_f)}(\mu_h^2)$ the operator matrix elements (partially known up to N^{3}LO)

for backward evolution:

- invert $\tilde{\mathbf{E}}^{(n_f)}$: simple
- invert $\mathbf{R}^{(n_f)}$: simple
- invert $\tilde{\mathbf{A}}^{(n_f)}$: expanded or exact

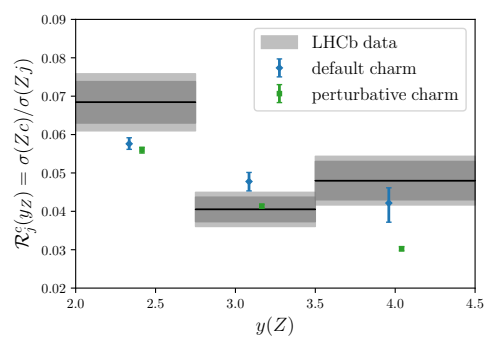
Intrinsic Charm: PDF plot



[BHPS] or [Meson/Baryon Cloud Model]

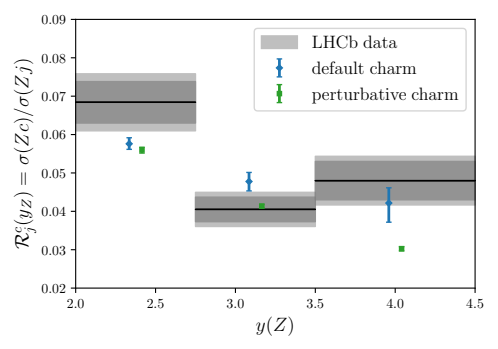
- in **3FNS** a valence-like peak is present
- for $x \leq 0.2$ the perturbative uncertainties are quite large
- the carried momentum fraction is within **1%**

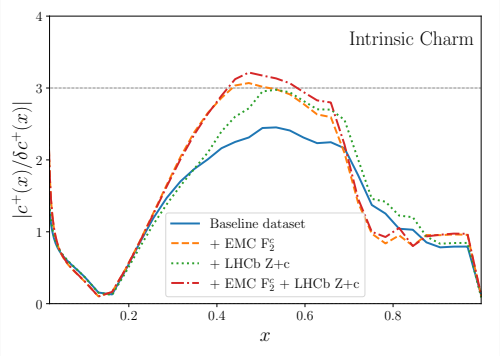
Intrinsic Charm: LHCb and Significance



- match better recent **LHCb** Z+c measurement [PRL128.082001]

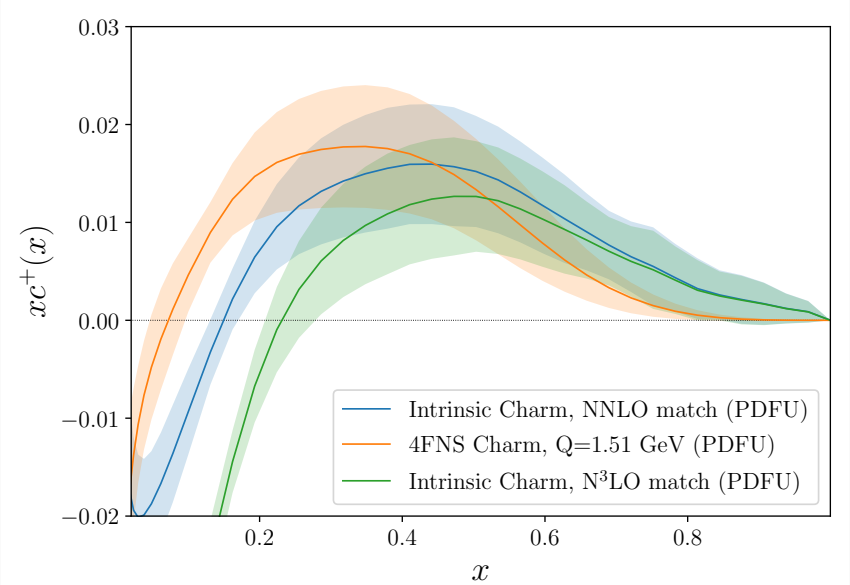
Intrinsic Charm: LHCb and Significance



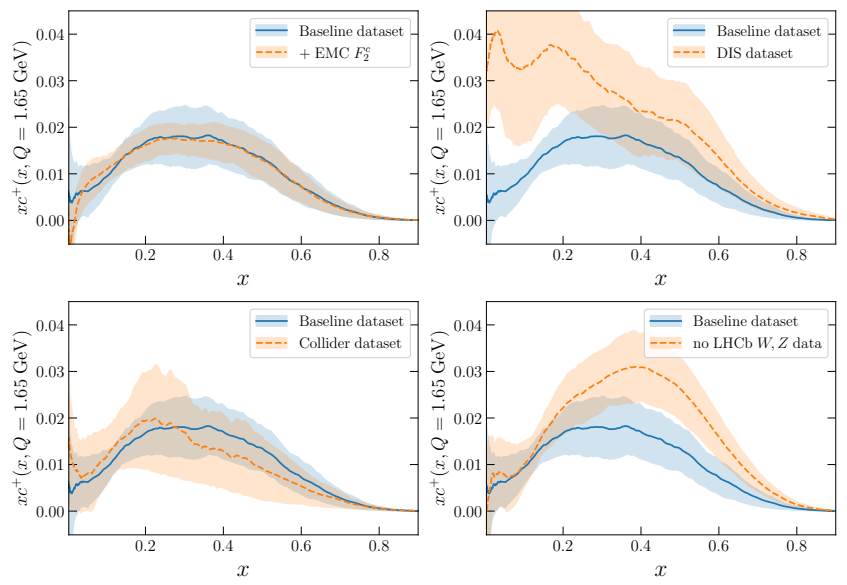


- match better recent **LHCb** Z+c measurement [PRL128.082001]
- we find a **3σ** evidence of intrinsic charm
- result is **stable** with mass variation, dataset variation

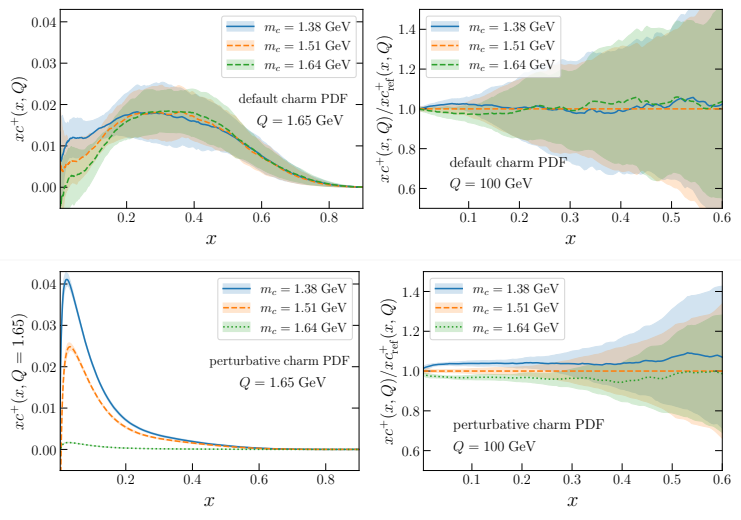
IC - uncertainties splitted



IC - dataset variation



IC - mass variation

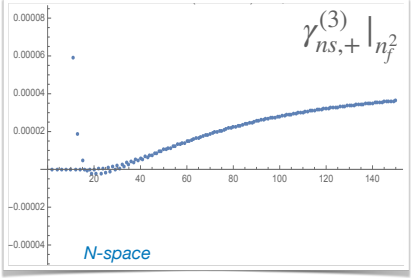


N3LO non singlet sector

non-singlet 4-loop Anomalous Dimensions

	n_f^0	n_f^1	n_f^2	n_f^3
$\gamma^{(3)}_{ns,-}$	✓	✓	✓	✓
$\gamma^{(3)}_{ns,+}$	✓	✓	✓	✓
$\gamma^{(3)}_{ns,s}$		✓	✓	

Comparison w.r.t. known analytical part (%)

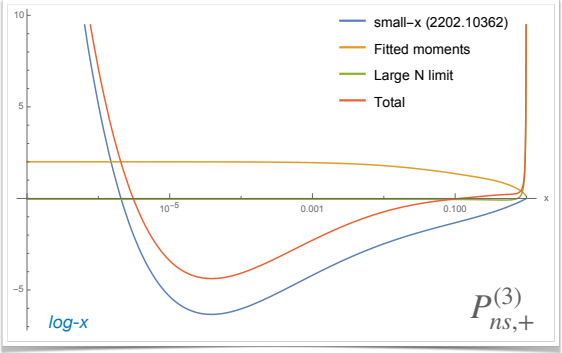


Main references:

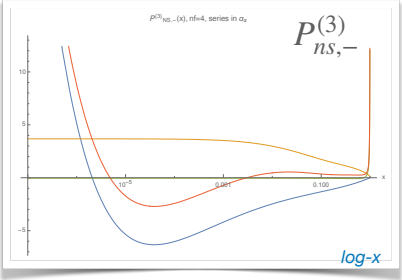
- Moch, Ruijl, Ueda, Vermaseren, Vogt [arXiv:1707.08315].
- Davies, Vogt, Ruijl, Ueda, Vermaseren. [arXiv:1610.07477]
- Davies, Kom, Moch, Vogt . [arXiv:2202.10362].

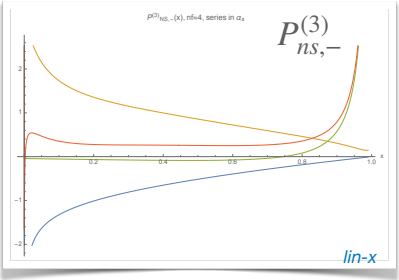
Rule of thumb:
small-N → small-x,
large-N → large-x

- Estimation of the N3LO anomalous dimensions is based on the best available theoretical constraints:
  - large-N:
  $$\gamma^{(3)}_{ns}(N\to\infty) \approx \Gamma_f S_1(N) + B + C\frac{S_1(N)}{N} + D\frac{1}{N} + \mathcal{O}(\frac{\ln(N)}{N^2})$$
  - small-N:
  $$\gamma^{(3)}_{ns}(N\to 0) \approx \sum_{i=1}^{7} C_i \frac{1}{N^i}$$
  - 8 lowest Mellin moments
- For more details on the procedure used see EKO N3LO ad documentation
- Non singlet approximated spitting functions are compatible with the known analytical (and much more complex) parts within numerical accuracy.



N3LO non singlet





- small−x (2202.10362)
- Fitted moments
- Large N limit
- Total