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Towards an NLO EW PDF fit with NNPDF and PineAPPL arXiv:2008.12789

Christopher Schwan

with: Stefano Carrazza, Emanuele R. Nocera, Marco Zaro

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Introduction					
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The race for precision at the LHC: Experiment, Theory, PDFs

- No spectacular deviations from SM predictions at the LHC
- LHC Run-1: $\sqrt{s} = 7 \text{ TeV}$ and $\sqrt{s} = 8 \text{ TeV}$
- LHC Run-2: $\sqrt{s} = 13 \, {
 m TeV}$, $L pprox 140 \, {
 m fb}^{-1}$
- $\mathsf{N}^2\mathsf{LO}$ QCD for all $2\to 2$ and a few $2\to 3$ processes
- automated NLO EW calculations
- resummations for specific observables up to N³LL
- small(er) theoretical/experimental uncertainties, stringent tests of the SM
- PDF determinations profit from this and own developments, e.g. better fitting methodologies
- \rightarrow better understanding of the structure of the proton (e.g. *reliably* smaller PDF uncertainties)



Plot from [ATLAS Collaboration]

Introduction			
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Plot from [ATLAS Collaboration]

Introduction					
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Why better understand proton PDFs?

- PDFs interesting on their own, but ...
- contributes to theory uncertainty of observables
- e.g. N³LO Higgs (right side) with [PDF4LHC15]
- $\delta(\mathsf{PDF} + \alpha_{\mathsf{s}})$: relative PDF and α_{s} uncertainty
- $\delta(\text{PDF-TH}):$ perturbative uncertainty from using $N^2\text{LO}$ PDFs and $N^3\text{LO}$ calculation

$$\delta(\mathsf{PDF-TH}) = \frac{1}{2} \left| \frac{\sigma(\mathsf{NNLO}) - \sigma(\mathsf{NLO})}{\sigma(\mathsf{NNLO})} \right|$$



plot from [F. Dulat, A. Lazopoulos, B. Mistlberger]

- \bullet or ATLAS 7 TeV $M_{\rm W}$ measurement, δm_W [MeV] with $_{\rm [CT10NNLO]}$
- or any other LHC observable...

W-boson charge	W	7+	W	7-	Com	oined
Kinematic distribution	p_T^ℓ	$m_{\rm T}$	p_T^ℓ	$m_{\rm T}$	p_T^ℓ	m_{T}
$\delta m_W [MeV]$						
Fixed-order PDF uncertainty	13.1	14.9	12.0	14.2	8.0	8.7
AZ tune	3.0	3.4	3.0	3.4	3.0	3.4
Charm-quark mass	1.2	1.5	1.2	1.5	1.2	1.5
Parton shower μ_F with heavy-flavour decorrelation	5.0	6.9	5.0	6.9	5.0	6.9
Parton shower PDF uncertainty	3.6	4.0	2.6	2.4	1.0	1.6
Angular coefficients	5.8	5.3	5.8	5.3	5.8	5.3
Total	15.9	18.1	14.8	17.2	11.6	12.9

table from [ATLAS Collaboration]

Introduction					
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NNPDF4.0: A much more precise/accurate PDF set

- See talks at:
 - PDF4LHC: https://indi.to/sc8mQ
 - DIS: https://www.stonybrook.edu/cfns/dis2021/
 - LoopFest/Radcor: https://indi.to/5Q6G8
- hyperoptimised fitting methodology, more LHC data, nuclear uncertainties, ... see Emanuele R. Nocera's talk at DIS 20201: https://indi.to/F8cFg
- stronger tests: closure test, future test [J. Cruz-Martinez, S. Forte, E.R. Nocera]
- ightarrow goal: \lesssim 1 % uncertainties in luminosities, integrated/differential cross sections:



[ABMP16], [CT18], [MSHT20], [NNPDF3.1], [NNPDF3.1str]

Introduction					
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Beyond NNPDF4.0: EW corrections

- NNPDF4.0 aims for $\leq 1\%$ accuracy/precision
- Further improvement need previously neglected contributions: theory uncertainties, NLO EW, ...
- NLO EW: never been done in a global (all processes) and consistent way (correct data)



- Can include extreme phase-space regions with large EW corrections: large $M_{\ell\ell}$ in Drell–Yan, large $p_{\rm T}$ of Z/W bosons, ... \rightarrow constrain high x
- These regions are going to be measured more precisely in the future, e.g. predictions for CMS DY L = 2.8 fb⁻¹ @ 13 TeV [CMS Collaboration]



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NLO EW in a PDF fit: What needs to be done?

- ✓ Photon-PDF: use NNPDF-LUXQED technology [NNPDF Collaboration], [A. Manohar et al.], [A. Manohar et al.]
- ✓ QED corrections in DGLAP with APFEL [V. Bertone, S. Carrazza, J. Rojo]
- ✓ Theory: Need corrections in the form of interpolation grids: PineAPPL
 - interfaced with MG5_aMC@NLO, see [S. Carrazza, E.R. Nocera, C.S., M. Zaro]; now released in v3.1.0: https://launchpad.net/mg5amcnlo
 - WIP: SHERPA/MCgrid [E. Bothmann et al.]
 - API available in C, C++, Fortran, Python, Rust
- ✓ Write/test runcards for all PDF processes and
- X Run them (WIP)
- ✓ Data: Needs careful selection
 - no subtraction of FSR
 - no photon-initiated subtraction
 - proper observable definition
 - \rightarrow subset of NNPDF4.0's LHC data + ...
 - \rightarrow DIS data?
- X Implement changed data (WIP)
- \rightarrow Run fit

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What is PineAPPL?

PineAPPL

A tool/library for storing PDF-independent theoretical predictions in interpolation grids [S. Carazza, E.R. Nocera, C.S., M. Zaro]



- write runcards for your process/distributions
- Ø MC generates histograms with PDFs baked-in
- Schanging PDFs is slow—need to rerun everything

Alternatively:

- on-the-fly evaluation of PDFs (typically one PDF set)
- reweighting





grids can be convolved with arbitrary PDF sets in a matter of seconds

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Interpolation techniques and applications

Well-known idea:

- APPLgrid [T. Carli et al.] or
- fastNLO [T. Kluge, K. Rabbertz, M. Wobisch]

Interpolate PDFs $f_a(x)$ with Lagrange polynomials $L_i(x), x \mapsto (0, 1)$:

$$f_a(x,Q^2) = \sum_{i=1}^\infty f^a_{ij}L_i(x)L_j(Q^2), \hspace{1em} f^a_{ij} \in \mathbb{R}$$

Convolution turns into a sum:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\mathcal{O}} = \sum_{a} \int \mathrm{d}x \int \mathrm{d}Q^2 f_a(x,Q^2) \frac{\mathrm{d}\sigma_a}{\mathrm{d}\mathcal{O}}(x,Q^2) = \sum_{aij} f_{ij}^a G_{ij}^a$$

Interpolation grid $\{G_{ii}^a\}_{aij}$ independent of PDFs:

$$G_{ij}^{a} = \int \mathrm{d}x \int \mathrm{d}Q^2 \, L_i(x) L_j(Q^2) \sigma_a(x,Q^2)$$

The price we have to pay:

- Interpolation error: typically sub-per mille
- Grids can become quite large (100 MB to 1000 MB)

Why PineAPPL?

- \rightarrow need support EW corrections (any powers of α and/or α_s)
- performance becomes very important: more bins, initial-states, scale variations . . .
- better tooling (see later slides)

Applications of interpolation grids

- study impact of PDFs uncertainties of observables or
- input for PDF fits

Interpolation grids		
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Interpolation grids as input for PDF fits



• calculate interpolation grids G_{ijk}^{ab} for

many process (shown is ATLAS DY high-mass 7 TeV [ATLAS Collaboration])

- parametrise PDFs f^a_{ij} (neural networks)
- get the corresponding measurements D_n and experimental covariancee matrix C_{nm}
- calculate theory predictions T_n for all observables of all experiments

(a) calculate χ^2

o update PDF parameters

Image: Image

	Interpolation grids				
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How does an interpolation grid look like: $\mathcal{O}(\alpha_s^2 \alpha) / \mathcal{O}(\alpha_s^2)$ for $gg \to t\bar{t}$ @ 8 TeV





- integrated correction of ${\cal O}(\alpha_{\rm s}^2\alpha)/{\cal O}(\alpha_{\rm s}^2)$ roughly $-0.5\,\%$
- corrections differential in x_1 and x_2

• y: bin indices;
$$y = 0 \mapsto x = 1$$
, $y = 50 \mapsto x_{\min} = 10^{-7}$

- $y_a \leftrightarrow y_b$ symmetry: initial-state symmetry of $\mathrm{gg} \to \mathrm{t} \overline{\mathrm{t}}$
- lower left corner \rightarrow production threshold at $8\,\text{TeV}\cdot\sqrt{x_1x_2}>2m_{\rm t}$
- at threshold: Coulomb singularity
- negative correction for larger x_a , x_b
- no interpolation in y_a , y_b , or Q^2
 - $y_{a/b}(x) \propto -\ln x_{a/b} + 5(1 x_{a/b})$

	Interpolation grids				
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Alternative: K factors + NLO QCD interpolation grids

Sometimes it's not possible to generate higher-order interpolation grids; use K factors:

$$K_{\rm NNLO} = \frac{{\rm d}\sigma_{\rm NNLO}/{\rm d}\mathcal{O}}{{\rm d}\sigma_{\rm NLO}/{\rm d}\mathcal{O}} \qquad K_{\rm EW} = \frac{{\rm d}\sigma_{\rm EW}/{\rm d}\mathcal{O}}{{\rm d}\sigma_{\rm QCD}/{\rm d}\mathcal{O}} \qquad \frac{{\rm d}\sigma^{\rm NNLO}}{{\rm d}\mathcal{O}} \approx \sum_{aii} K_{\rm NNLO} f^a_{ij} G^{a,\rm NLO}_{ij}$$

- NNPDF (and ABMP, CT, MSHT) use NNLO QCD K_{NNLO} factors instead of interpolation grids
- MSHT20 uses K_{EW} factors for some NLO EW corrections

Features of K factors:

- very easy to handle, especially if MCs aren't public
- if $K \approx 1$, they won't impact the PDF fit
- however: K factors are blind to initial-state parton flavours, x_1, x_2 and Q^2
- $\rightarrow\,$ new partonic channels opening up NNLO or NLO EW are zero!
- \rightarrow K = 1 and massive reshuffling between flavours/scales?

Goals:

- For NLO EW we chose interpolation grids to be on the safe side
- We want to switch from NNLO QCD K factors to grids at some point

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Which EW corrections will be included for $pp \rightarrow \ell \bar{\ell}$?





• NNLO QCD corrections included in PDF fits

- ightarrow include also higher-order lpha contributions in NNPDF 4.×
 - for all processes
 - check impact of the corrections,
 - be more inclusive, etc.
- → PineAPPL supports all higher-orders
- $\mathcal{O}(lpha_{
 m s} lpha^3)$ might become available at some point . . .

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	EW corrections		
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			Data issues		
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Lepton observables: what do we call a lepton?

Basic lepton facts:

- very important for PDF processes: DY, W boson prod., Z-boson $p_{\rm T}, \ldots$
- they radiate: lots of collinear and/or soft photons!
- in NNLO QCD: no additional photon radiation
- in NLO EW: up to one extra photon
- ightarrow we must be able to calculate what is being measured; understand lepton definition!

Three possible definitions for 'lepton'

- Only charged object is the lepton: bare lepton
- **2** Add photons around some ΔR of the lepton: dressed lepton
- Lepton before it radiates: Born lepton



			Data issues		
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Which lepton observable definition do we adopt?



- bare leptons: non-collinear safe, useful for muons, see e.g. [S. Dittmaier, A. Kabelschacht, T. Kasprzik]
- Born leptons: leptons "before they radiate", calculated using shower inversion (PHOTOS), from
- ightarrow dressed leptons: leptons with photons recombined around $\Delta R_{f\gamma}$, typically $\Delta R_{f\gamma}=0.1$
- dressing factors

$$\mathcal{C}_{\mathsf{dress}} = rac{\mathrm{d}\sigma_{\mathsf{dressed}}/\mathrm{d}\mathcal{O}}{\mathrm{d}\sigma_{\mathsf{Born}}/\mathrm{d}\mathcal{O}}$$

can be very large, up to 50 % in invariant mass distributions

- Born leptons for comparisons with QCD-only theory predictions
- \rightarrow dressed leptons for comparisons with EW (+QCD) corrections
- For some analyses dressed-lepton data not published: double counting issue with Born-lepton data!
- ightarrow NLO EW PDF dataset largely determinedy by whether dressed-lepton dataset is available; sometimes we can't tell

			Data issues		
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Effects of FSR in Drell-Yan: CMS 13 TeV $L = 2.8 \text{ fb}^{-1}$ [CMS Collaboration]



- large corrections of the NLO EW around the Z peak: QED FSR
- very large if bins are small (LHC run II feature)
- probably calls for resummation
- subtracted in data in pre-FSR datasets
- scale-variation band much larger: interplay with theory uncertainties in PDF?
- not described by FSR: weak corrections for large $M_{\ell\ell}$ \rightarrow need full EW corrections
- dressed-lepton data sometimes not available

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Subtraction of photon-photon contribution



- For ATLAS and CMS it seems to be standard procedure to subtract double-photon induced contributions: The photon-induced process, $\gamma\gamma \rightarrow \ell \bar{\ell}$, is simulated at LO using Pythia 8 and the MRST2004ged PDF set.
- not considered part of "Drell-Yan lepton pair production"
- Problem for our exercise: proton contains photons, should be counted towards signal!
- Subtracted in data, original data most likely lost
- $\bullet\,$ Size of the LO contribution can become significant in large-invariant-mass bins (3 % to 6 %) depending on the used PDF

	Data issues	
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Z transverse momentum

$$\begin{array}{c} \mathbf{q} & \mathbf{Z}, \gamma & \mu^+ \\ \mu^- & \mu^- \end{array} \qquad \mu = \sqrt{M_{\mathbf{Z}}^2 + (\mathbf{p}_{\mathbf{T}}^{\ell\bar{\ell}})^2} \end{array}$$

- FSR issues similar to DY, but typically 60 GeV $< M_{\ell\bar{\ell}} <$ 120 GeV \rightarrow small QED corrections
- plot on the RHS: predictions for CMS 13 TeV $L = 35.8 \text{ fb}^{-1}$ [CMS Collaboration]
- compare size of NLO EW (blue) vs. data uncertainty (gray)
- no photon subtraction (small contribution)
- \rightarrow large weak corrections at large transverse momentum, similar to data uncertainty (with $L=35.8\,{\rm fb}^{-1})$
- \bullet use a resummed prediction for $p_{\rm T} < 30\,{\rm GeV}\colon$ very precise data



			Data issues		
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t-channel single-top production

Not properly/easily definable at NLO EW (see also [R. Frederix, D. Pagani, I. Tsinikos]):

- will be included in NNPDF4.0 for the first time
- Analyses, e.g. [ATLAS collaboration], treat s-channels as irreducible background
- single-production at LO:



• but at NLO EW not (gauge-invariantly) separable:



- $\rightarrow\,$ ignore these datasets
- better idea: partonic cross section with zero b jets?
- probably not too important [E.R. Nocera, M. Ubiali, C. Voisey], due to larger data uncertainty

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How can I play with PineAPPL?

- Install Madgraph5_aMC@NLO (at least v3.1.x): https://launchpad.net/mg5amcnlo
- Install PineAPPL: https://github.com/N3PDF/pineappl
- Example for generating the DY plot (next page) available at https://github.com/N3PDF/pineappl/tree/master/examples/mg5amcnlo

- only one line needs to be added in the mg5amc runcard (rhs)
- No two-phase generation of the grids needed
- Replaces the aMCfast [V. Bertone et al.] interface in Madgraph5_aMC@NLO v2.x
- PineAPPL's CLI allows to easily produce convolutions and plots

```
launch processname
[..]
set ptl = 25.0
set etal = 2.5
set mll_sf = 116
set req_acc_F0 0.001
set pineappl True
done
quit
```

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PineAPPL: --help

```
$ pineappl --help
pineappl 0.5.0-alpha
Read, write, and guery PineAPPL grids
USAGE :
    pineappl [FLAGS] <SUBCOMMAND>
FLAGS:
    -h. --help
                            Prints help information
        --silence-lhapdf
                            Prevents LHAPDF from printing banners
    -V. --version
                            Prints version information
SUBCOMMANDS :
    channels
                       Shows the contribution for each partonic channel
    convolute
                       Convolutes a PineAPPL grid with a PDF set
    diff
                       Compares the contents of two grids with each other
                       Shows information about the grid
    info
                       Shows the luminosity function
    luminositv
                       Merges one or more PineAPPL grids together
    merge
                       Optimizes the internal data structure to minimize memory usage
    optimize
                       Shows the predictions for all bin for each order separately
    orders
    pdf uncertainty
                       Calculates PDF uncertainties
    plot
                       Creates a matplotlib script plotting the contents of the grid
                       Modifies the bin dimensions, widths and normalizations
    remap
                       Modifies the internal key-value storage
    set
    subgrids
                       Print information about the internal subgrid types
                       Sums two or more bins of a grid together
    sum
```

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pineappl.lz4 \

PineAPPL: convolute

\$	pin	neappl	cor	volute NNPDF	F_DY_14TEV	/_40_PHENO
>	NNF	PDF31_	nlo_	as_0118_luxq	leq	
bi	n	M11		dsig/dMll	neg unc	pos unc
	- + -	+-	+		+	
	0	40	45	2.5430906e0	-6.34%	4.43%
	1	45	50	2.1991339e0) -7.05%	4.57%
	2	50	55	1.9127949e0) -7.45%	4.86%
	3	55	60	1.7689139e0) -7.85%	5.37%
	4	60	64	1.7440995e0	-8.20%	5.87%
	5	64	68	1.8550755e0	-8.49%	6.30%
	6	68	72	2.1362930e0	-8.71%	6.63%
	7	72	76	2.7074748e0	-8.69%	6.69%
	8	76	81	4.1704013e0	-8.40%	6.44%
	9	81	86	9.4844889e0	-7.47%	5.51%
1	0	86	91	7.0167791e1	-4.99%	2.88%
1	1	91	96	7.7155277e1	-3.79%	1.68%
1	2	96	101	6.8573762e0) -3.79%	1.86%
1	3	101	106	2.3582461e0) -3.72%	1.94%
1	4	106	110	1.2757496e0	-3.67%	2.01%
1	5	110	115	8.1275105e-1	-3.51%	1.95%
1	6	115	120	5.4706411e-1	-3.43%	1.98%
1	7	120	126	3.8159272e-1	-3.20%	1.83%
1	8	126	133	2.6919040e-1	-3.15%	1.92%
1	9	133	141	1.9164180e-1	-2.97%	1.83%
2	20	141	150	1.3594679e-1	-2.75%	1.74%
2	21	150	160	9.7852913e-2	2 -2.55%	1.63%
2	22	160	171	7.1471465e-2	2 -2.48%	1.68%
2	23	171	185	5.1601085e-2	2 -2.35%	1.67%

- bin: bin index
- Mll: lower and upper limit of $M_{\ell\bar{\ell}}$ bin
- dsig/Mll: differential cross section for the bin
- neg unc/textttpos unc: 7-point scale variation uncertainty

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PineAPPL: plot



```
$ pineappl --silent-lhapdf plot \
    DY_14.pineappl.l24 \
    210219-01-rs-nnpdf40-baseline \
    MSHT20nnlo_asi18 \
    CT18NNLD \
    ABMP16alsi18_5_nnlo > plot.py
$ python3 plot.py
```

- generates self-contained matplotlib script (can be modified easily)
- absolute predictions
- NLO EW on vs. NLO EW off (relative)
- PDF uncertainties fo
 - NNPDF 4.0 candidate fit
 - MSHT20
 - CT18 (only main set)
 - ABMP16
- pull: weighted difference w.r.t. NNPDF 4.0 in units of σ

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PineAPPL: plot



```
$ pineappl --silent-lhapdf plot \
    DY_14.pineappl.lz4 \
    210219-01-rs-nnpdf40-baseline \
    MSHT20nnlo_asi18 \
    CT18NNLO \
    ABMP16alsi18_5_nnlo > plot.py
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PineAPPL: channels

<pre>\$ pineappl luminosity \</pre>	\$ p	ineapp	ol cha	annels	NNPDF.	_DY_14	1TEV_40	_PHENO	.pineapp	ol.lz4	\
> NNPDF_DY_14TEV_40_PHENO.pineappl.lz4	> N1	NPDF3	1_nlo.	_as_01	l18_luxo	qed -·	-limit ·	4			
id entry entry entry	bin	MI	11	lumi	size	lumi	size	lumi	size	lumi	size
+		+	+	++		+		++		+	
#0 1 x (2, -2) 1 x (4, -4)	14	106	110	#5	58.28%	#0	48.56%	#10	5.06%	#7	-3.12%
#1 1 x (22, -4) 1 x (22, -2)	15	110	115	#5	56.55%	#0	50.12%	#10	4.85%	#7	-2.97%
#2 1 x (0, -4) 1 x (0, -2)	16	115	120	#5	54.32%	#0	51.64%	#10	4.58%	#7	-2.75%
#3 1 x (2, 22) 1 x (4, 22)	17	120	126	#0	53.05%	#5	52.82%	#10	4.42%	#7	-2.67%
#4 1 x (2, 0) 1 x (4, 0)	18	126	133	#0	54.51%	#5	50.62%	#10	4.11%	#2	-2.47%
#5 1 x (1, -1) 1 x (3, -3)	19	133	141	#0	56.39%	#5	48.56%	#10	3.93%	#2	-2.47%
#6 1 x (22, -3) 1 x (22, -1)	20	141	150	#0	57.07%	#5	47.26%	#10	3.78%	#15	2.61%
#7 1 x (0, -3) 1 x (0, -1)	21	150	160	#0	59.31%	#5	45.00%	#10	3.46%	#15	2.79%
#8 1 x (1, 22) 1 x (3, 22)	22	160	171	#0	60.02%	#5	43.35%	#10	3.36%	#15	3.12%
#9 1 x (1, 0) 1 x (3, 0)	23	171	185	#0	60.78%	#5	42.28%	#15	3.48%	#10	3.05%
#10 1 x (5, -5)	24	185	200	#0	62.90%	#5	40.28%	#15	3.57%	#10	2.77%
#11 1 x (22, -5)	25	200	220	#0	62.25%	#5	40.38%	#15	3.87%	#10	2.76%
#12 1 x (0, -5)	26	220	243	#0	64.55%	#5	37.83%	#15	3.87%	#4	-2.50%
#13 1 x (5, 22)	27	243	273	#0	65.04%	#5	36.77%	#15	4.04%	#4	-2.37%
#14 1 x (5, 0)	28	273	320	#0	66.25%	#5	35.56%	#15	4.44%	#4	-2.77%
#15 1 x (22, 22)	29	320	380	#0	67.41%	#5	33.93%	#15	4.65%	#4	-2.72%
#16 1 x (-5, 22) 1 x (-3, 22) 1 x (-1, 22)	30	380	440	#0	68.82%	#5	32.79%	#15	4.15%	#4	-2.88%
#17 1 x (1, 22) 1 x (3, 22) 1 x (5, 22)	31	440	510	#0	68.22%	#5	32.32%	#15	4.83%	#4	-2.72%
	32	510	600	#0	70.50%	#5	30.18%	#15	4.65%	#4	-2.86%
a 0 — un sucedu 0 — sluces 00 — shates	33	600	700	#0	70.40%	#5	29.92%	#15	4.64%	#4	-2.60%
• $2 = up$ quark, $0 = gluon$, $22 = photon$,	34	700	830	#0	71.47%	#5	28.59%	#15	4.52%	#4	-2.35%
(22 22): # 15 $\alpha \alpha$ initial state	35	830	1000	#0	72.87%	#5	27.30%	#15	4.45%	#4	-2.94%
• (22, 22). π 13, π initial state	36	1000	1500	#0	75.13%	#5	25.33%	#15	4.56%	#4	-3.34%
	37	1500	3000	#0	76.19%	#5	21.76%	#15	6.43%	#4	-2.84%

		Conclusions
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Summary

- NLO EW corrections for PDF fits: upgrading the precision of PDF processes
- PineAPPL: interpolation tool/library for storing PDF-independent theoretical predictions https://github.com/N3PDF/pineappl
- Built-in support in Madgraph5_aMC@NLO v3.1.0
- data issues: FSR subtraction, photon-initiated subtraction,
- $\rightarrow\,$ effectively determines the datasets we can use for the fit

Outlook:

- We will publish grids for ATLAS/CMS/LHCb analyses (PDF processes) soon
- \rightarrow PineAPPL already public and Open Source: https://n3pdf.github.io/pineappl
- NLO EW PDF fit not too far away