#### APPLgrid news

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# Proton-proton collision



hard scattering can be calculated to NLO(NNLO) precision

- description of showers and non-perturbative effects comes from MC
- PDFs and strong coupling are determined from precision data (LEP, HERA, TEVATRON, ...).

## N<sup>x</sup>LO QCD cross section



$$\frac{d\sigma}{dX} \sim \sum_{(i,j,p)} \int d\Gamma \alpha_s^p(Q_R^2) \ q_i(x_1, Q_F^2) q_j(x_2, Q_F^2) \ \frac{d\hat{\sigma}_{(p)}^{ij}}{dX}(x_1, x_2, Q_F^2, Q_R^2; \ S)$$

- Coupling and parton density functions are non-perturbative inputs to calculation (extracted from data)
- Perturbative coefficients are essentially independent from PDF functions due to factorization theorem

Calculating NLO cross-sections takes a long time ( $\sim days/weeks/months$ )

 $\implies$  we can split calculation into two parts

#### APPLGRID method

- Step 1 (long run): Collect perturbative weights to grids .
  - binning
  - interpolation
  - ▶ initial flavours decomposition :  $13 \times 13 \rightarrow \mathcal{L}$ ( $\mathcal{L} \sim 10$ )

$$\frac{d\hat{\sigma}_{(p)}^{ij}}{dX}(x_1, x_2, Q_F^2, Q_R^2; S) \xrightarrow{3D-grid} w^{(p)(l)}(x_1^m, x_2^n, Q^{2^k}) (Q_R^2 \equiv Q_F^2)$$

- Step 2 ( $\sim$  10–100 ms): Convolute grid with PDF's .
  - ▶ integral → sum
  - any coupling, PDF

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## Details of the method (I)

Interpolation

• user defined interpolation orders  $n_y$ ,  $n_\tau$ 

$$f(x, Q^2) = \sum_{i=0}^{n_y} \sum_{\iota=0}^{n_\tau} f_{k+i,\kappa+\iota} I_i^{(n)} \left(\frac{y(x)}{\delta y} - k\right) I_i^{(n')} \left(\frac{\tau(Q^2)}{\delta \tau} - \kappa\right)$$

#### Subprocess decomposition

 $13\times13\rightarrow\mathcal{L}$  due to the symmetries of the ME weights

$$\sum_{m,n} \nu_{mn}^{(l)} f_{m/H_1}\left(x_1, Q^2\right) f_{n/H_2}\left(x_2, Q^2\right) \equiv F^{(l)}\left(x_1, x_2, Q^2\right),$$

"generalised" PDFs depend on the process and the perturbative order

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#### APPLGRID subprocesses for $W^{\pm}$ production (I)



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#### APPLGRID subprocesses for $W^{\pm}$ production (II)

The weights for  $W^+$ -production can be organized in six possible initial state combinations (calculated using MCFM)

$$\begin{split} \bar{D}U : & F^{(0)}\left(x_{1}, x_{2}, Q^{2}\right) = \sum_{j=1,3,5} f_{-j/H_{1}}\left(x_{1}\right) \sum_{i=2,4,6} f_{i/H_{2}}\left(x_{2}\right) V_{ij}^{2} \\ U\bar{D} : & F^{(1)}\left(x_{1}, x_{2}, Q^{2}\right) = \sum_{i=2,4,6} f_{i/H_{1}}\left(x_{1}\right) \sum_{j=1,3,5} f_{-j/H_{2}}\left(x_{2}\right) V_{ij}^{2} \\ \bar{D}g : & F^{(2)}\left(x_{1}, x_{2}, Q^{2}\right) = \sum_{i=1,3,5} f_{-i/H_{1}}\left(x_{1}\right) \left(V_{iu}^{2} + V_{ic}^{2} + V_{it}^{2}\right) f_{0/H_{2}}\left(x_{2}\right) \end{split}$$

$$Ug: \qquad F^{(3)}\left(x_{1}, x_{2}, Q^{2}\right) = \sum_{i=2,4,6} f_{i/H_{1}}\left(x_{1}\right) \left(V_{id}^{2} + V_{is}^{2} + V_{ib}^{2}\right) f_{0/H_{2}}\left(x_{2}\right)$$

$$g\bar{D}: \qquad F^{(4)}\left(x_{1}, x_{2}, Q^{2}\right) = \sum_{i=1,3,5} f_{0/H_{1}}\left(x_{1}\right) \left(V_{iu}^{2} + V_{ic}^{2} + V_{it}^{2}\right) f_{-i/H_{2}}\left(x_{2}\right)$$

$$gU: \qquad F^{(5)}\left(x_{1}, x_{2}, Q^{2}\right) = \sum_{i=2,4,6} f_{0/H_{1}}\left(x_{1}\right) \left(V_{id}^{2} + V_{is}^{2} + V_{ib}^{2}\right) f_{i/H_{2}}\left(x_{2}\right)$$

We separate  $u\bar{d}$  from  $\bar{d}u$  in order to get the right rapidity distribution for the electron,

because of the chiral nature of the  $W^{\pm}$  couplings

APPLGRID project

#### APPLGRID subprocesses for $Z^0$ production We can introduce 12 sub-processes in Z production (calculated using

MCFM)

	UŪ :	${{m {F}}^{(0)}}\left( {{m x_1},{m x_2},{m Q}^2}  ight) = {m U_{12}}({m x_1},{m x_2})$
	<b>D</b> <i>D</i> :	$F^{(1)}(x_1, x_2, Q^2) = D_{12}(x_1, x_2)$
	<i>ŪU</i> :	$F^{(2)}\left(x_{1},x_{2},Q^{2} ight)=U_{21}(x_{1},x_{2})$
	<b>D</b> D :	$F^{(3)}\left(x_{1},x_{2},Q^{2} ight)=D_{21}(x_{1},x_{2})$
	<b>gU</b> :	$F^{(4)}\left(x_{1},x_{2},Q^{2} ight)=G_{1}(x_{1})U_{2}(x_{2})$
i from <i>ūu</i>	$gar{U}$ :	$\mathcal{F}^{(5)}\left(x_1,x_2,Q^2 ight)=G_1(x_1)\overline{U}_2(x_2)$
include e	<b>gD</b> :	${\cal F}^{(6)}\left(x_1,x_2,Q^2 ight)=G_1(x_1)D_2(x_2)$
	<b>g</b> D :	$\mathcal{F}^{(7)}\left(x_1,x_2,Q^2 ight)=G_1(x_1)\overline{D}_2(x_2)$
	<b>Ug</b> :	$F^{(8)}\left(x_{1},x_{2},Q^{2} ight)=U_{1}(x_{1})G_{2}(x_{2})$
	Ūg :	$\mathcal{F}^{(9)}\left(x_1,x_2,Q^2 ight)=\overline{U}_1(x_1)\mathcal{G}_2(x_2)$
	<b>Dg</b> :	$F^{(10)}(x_1, x_2, Q^2) = D_1(x_1)G_2(x_2)$
	<i>D̄g</i> :	$F^{(11)}(x_1, x_2, Q^2) = \overline{D}_1(x_1)G_2(x_2)$
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We separate  $u\bar{u}$  from  $\bar{u}u$ contributions to include

 $\gamma/Z$  interference

#### APPLGRID subprocesses for $Z^0$ production II

Use is made of the generalised PDFs defined as:

$$\begin{split} & U_{H}(x) = \sum_{i=2,4,6} f_{i/H}\left(x,Q^{2}\right), \qquad \overline{U}_{H}(x) = \sum_{i=2,4,6} f_{-i/H}\left(x,Q^{2}\right), \\ & D_{H}(x) = \sum_{i=1,3,5} f_{i/H}\left(x,Q^{2}\right), \qquad \overline{D}_{H}(x) = \sum_{i=1,3,5} f_{-i/H}\left(x,Q^{2}\right), \\ & U_{12}(x_{1},x_{2}) = \sum_{i=2,4,6} f_{i/H_{1}}\left(x_{1},Q^{2}\right) f_{-i/H_{2}}\left(x_{2},Q^{2}\right), \\ & D_{12}(x_{1},x_{2}) = \sum_{i=1,3,5} f_{i/H_{1}}\left(x_{1},Q^{2}\right) f_{-i/H_{2}}\left(x_{2},Q^{2}\right), \\ & U_{21}(x_{1},x_{2}) = \sum_{i=2,4,6} f_{-i/H_{1}}\left(x_{1},Q^{2}\right) f_{i/H_{2}}\left(x_{2},Q^{2}\right), \\ & D_{21}(x_{1},x_{2}) = \sum_{i=1,3,5} f_{-i/H_{1}}\left(x_{1},Q^{2}\right) f_{i/H_{2}}\left(x_{2},Q^{2}\right), \end{split}$$

#### Details of the method (II) Phasespace optimisation



User just defines max/min possible values of x,  $Q^2$ . The optimisation procedure finds appropriate limits for each

subprocess/order/observable bin.

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 $\leftarrow$  x<sub>1</sub>x<sub>2</sub>-phasespace

#### Final result

$$\frac{d\sigma}{dX} = \sum_{p} \sum_{l=0}^{L} \sum_{m,n,k} w_{m,n,k}^{(p)(l)} \left(\frac{\alpha_s(Q_k^2)}{2\pi}\right)^{p_l} F^{(l)}\left(x_{1m}, x_{2n}, Q_k^2\right)$$

#### Scale dependence

Having the weights  $w_{m,n,k}^{(p)(l)}$  determined separately order by order in  $\alpha_s$ , it is straightforward to vary the renormalisation  $\mu_R$  and factorisation  $\mu_F$  scales a posteriori.

We assume scales to be equal

$$\mu_{R} = \mu_{F} = Q$$

in the original calculation.

Introducing  $\xi_R$  and  $\xi_F$  corresponding to the factors by which one varies  $\mu_R$  and  $\mu_F$  respectively,

$$\mu_R = \xi_R \times Q$$
$$\mu_F = \xi_F \times Q$$

#### Master formula and Scale dependence at NLO

Then for arbitrary  $\xi_R$  and  $\xi_F$  we may write:

$$\begin{aligned} \frac{d\sigma}{dX} & (\xi_{R},\xi_{F}) = \sum_{l=0}^{L} \sum_{m} \sum_{n} \sum_{k} \left\{ \left( \frac{\alpha_{s} \left( \xi_{R}^{2} Q^{2}_{k} \right)}{2\pi} \right)^{p_{\text{LO}}} \right)^{p_{\text{LO}}} \\ & \times W_{m,n,k}^{(\text{LO})(l)} F^{(l)} \left( x_{1\,m}, x_{1\,n}, \xi_{F}^{2} Q^{2}_{k} \right) + \left( \frac{\alpha_{s} \left( \xi_{R}^{2} Q^{2}_{k} \right)}{2\pi} \right)^{p_{\text{NLO}}} \\ & \times \left[ \left( W_{m,n,k}^{(\text{NLO})(l)} + 2\pi\beta_{0} p_{\text{LO}} \ln \xi_{R}^{2} W_{m,n,k}^{(\text{LO})(l)} \right) F^{(l)} \left( x_{1\,m}, x_{2n}, \xi_{F}^{2} Q^{2}_{k} \right) \\ & - \ln \xi_{F}^{2} W_{m,n,k}^{(\text{LO})(l)} \\ & \times \left( F_{q_{1} \rightarrow P_{0} \otimes q_{1}}^{(l)} \left( x_{1\,m}, x_{2n}, \xi_{F}^{2} Q^{2}_{k} \right) + F_{q_{2} \rightarrow P_{0} \otimes q_{2}}^{(l)} \left( x_{1\,m}, x_{2n}, \xi_{F}^{2} Q^{2}_{k} \right) \right) \right] \end{aligned}$$

where  $F_{q_1 \rightarrow P_0 \otimes q_1}^{(l)}$  is calculated as  $F^{(l)}$ , but with  $q_1$  replaced with  $P_0 \otimes q_1$  (LO splitting function convoluted with PDF), and analogously for  $F_{q_2 \rightarrow P_0 \otimes q_2}^{(l)}$ .

#### Master formula and Scale dependence at NNLO

$$\frac{d\sigma}{dX}(\xi_R,\xi_F) = \sum_{l=0}^{L} \sum_m \sum_n \sum_k F^{(l)}\left(x_{1m}, x_{2n}, \xi_F^2 Q_k^2\right) \times \left\{ \left(\frac{\alpha_s\left(\xi_R^2 Q_k^2\right)}{2\pi}\right)^{p_{\text{LO}}} W_{m,n,k}^{(\text{LO})(l)} + \left(\frac{\alpha_s\left(\xi_R^2 Q_k^2\right)}{2\pi}\right)^{p_{\text{NNLO}}} W_{m,n,k}^{(\text{NLO})(l)} + \left(\frac{\alpha_s\left(\xi_R^2 Q_k^2\right)}{2\pi}\right)^{p_{\text{NNLO}}} W_{m,n,k}^{(\text{NNLO})(l)} \right\} + \sum_{l=0}^{L} \sum_m \sum_n \sum_k \left(\frac{\alpha_s\left(\xi_R^2 Q_k^2\right)}{2\pi}\right)^{p_{\text{NNLO}}} \times \left\{ \text{Scale variations termS} \right\}$$

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Scale dependence at NNLO

$$L_R = \log \xi_R^2, \ L_F = \log \xi_F^2$$

$$= L_{R} \left( p_{\text{NLO}} \beta_{0} W_{m,n,k}^{(\text{NLO})(l)} + p_{\text{LO}} \beta_{1} W_{m,n,k}^{(\text{LO})(l)} \right) F^{(l)} \\ + L_{R}^{2} p_{\text{NLO}} \beta_{0}^{2} W_{m,n,k}^{(\text{LO})(l)} F^{(l)} \\ - L_{F} \left( W_{m,n,k}^{(\text{NLO})(l)} \left[ F_{q_{1} \rightarrow P_{0} \otimes q_{1}}^{(l)} + F_{q_{2} \rightarrow P_{0} \otimes q_{2}}^{(l)} \right] \\ + W_{m,n,k}^{(\text{LO})(l)} \left[ F_{q_{1} \rightarrow P_{1} \otimes q_{1}}^{(l)} + F_{q_{2} \rightarrow P_{1} \otimes q_{2}}^{(l)} \right] \right) \\ + L_{F}^{2} W_{m,n,k}^{(\text{LO})(l)} \left( F_{q_{1} \rightarrow P_{0} \otimes q_{1}; q_{2} \rightarrow P_{0} \otimes q_{2}} + \frac{1}{2} F_{q_{1} \rightarrow P_{0} \otimes P_{0} \otimes q_{1}}^{(l)} + \frac{1}{2} \beta_{0} F_{q_{1} \rightarrow P_{0} \otimes q_{1}}^{(l)} + \frac{1}{2} \beta_{0} F_{q_{1} \rightarrow P_{0} \otimes q_{1}}^{(l)} + \frac{1}{2} \beta_{0} F_{q_{2} \rightarrow P_{0} \otimes q_{2}}^{(l)} \right) \\ - L_{R} L_{F} p_{\text{NLO}} \beta_{0} W_{m,n,k}^{(\text{LO})(l)} \left( F_{q_{1} \rightarrow P_{0} \otimes q_{1}}^{(l)} + F_{q_{2} \rightarrow P_{0} \otimes q_{2}}^{(l)} \right)$$

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### APPLGRID accuracy.



## Scale variations validation



- Horizontal axis renormalisation scale
- Shaded bands factorisation scale variations from original NNLOJET paper
- Unshaded, hatched bands APPLgrid scale valuation

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### Changing PDFs and centre-of-mass-energy



Inclusive jet production

# Photon-induced processes

 Currently use a modification of the lhaglue type LHAPDF interface

```
extern "C" void evolvepdf(const doubles x, const doubles Q, double* x

xfx += 6;

for (int i = -6; i < 7; i++) xfx[i] = pdf->xfxQ(i, x, Q);

xfx[7] = pdf->xfxQ(22, x, Q);

}
```

- Use native LHAPDF 6 calls with call to access photon density, in Ihaglue type wrapper
- APPLgrid intrinsic lumi\_pdf class allows additional parton -7 or 22 for the photon



#### Interface to cross section calculators

- NLOJET++ : Jet production in  $pp(\bar{p})$  and ep collisions.
  - $\blacktriangleright~2 \rightarrow 2 \text{ and } 2 \rightarrow 3 \text{ at NLO}; 2 \rightarrow 4 \text{ at LO}$

www.desy.de/~znagy/Site/NLOJet++.htm.

 MCFM : parton-level NLO(NNLO) QCD cross sections calculator for various femtobarn-level processes at hadron-hadron colliders.

►  $V, V + nJet, V + b\bar{b}, VV, Q\bar{Q}, ... (~ O(300))$  mcfm.fnal.gov/

- SHERPA : Simulation of High-Energy Reactions of PArticles in lepton-lepton, lepton-photon, photon-photon, lepton-hadron and hadron-hadron collisions.
  - A huge amount of scattering processes sherpa.hepforge.org.
- aMC@NLO : A framework for the computation of hard events at the NLO or LO, to be subsequently showered (infrared-safe observables at the NLO or LO).
  - Matrix elements calculations from Madgraph 5 amcatnlo.web.cern.ch/amcatnlo/; madgraph.phys.ucl.ac.be/.
- DYNNLO : NNLO calculation of Drell-Yan processes at hadron colliders theory.fi.infn.it/grazzini/dy.html
- NNLOJET : NNLO calculation of vector boson, V+jet, Higgs, inclusive jet/dijet at hadron colliders

APPLGRID project

### Grid distribution: Ploughshare

#### ploughshare.web.cern.ch



#### Grid distribution: Ploughshare II

#### Full analysis records

Measurement of inclusive jet and dijet production in $pp$ collisions at $\sqrt{s}=7$ TeV using the ATLAS detector	÷	Full title and abstract Links to • Journal paper (DOI)
clusive jet and dijet cross sections have been measured in proton-proton collisions at a centre-of-mass energy of 7 TW using the ATLAS detector at the Large Hadron Collider. The cross sections were measured using jets clustered with the ami-KT algorithm with parameters IR-0.4 de-RoB. These measurements are based on the 2010 data sample, clossing of a statistic flagstate luminosity of 2 TW mean pickbars. Inclusive entropy of the section o		<ul> <li>Preprint</li> <li>Inspire</li> <li>HepData</li> <li>Table with all available grids</li> </ul>
vite a distribution in a region where they are currently not well-constrained. warnal: Phys. Rev. O&E (2012) 014022 (doi: 10.1103/PhysRev.0.86.014022)	Ċ	This information is determined automatically from the required preprin ID when you upload grids
sper: https://wpdate.net/record/002398 wpData:https://wpdata.net/record/no102398	) <sup>†</sup>	For grids with no corresponding paper, a dummy arrive number arxiv: 0000.00000 can be used
Ixperiment process energy Calculation direct link	•	Users will be able to provide an additional HTML fragment in the tgz file if they require
ITLAS pp 7 TeV NLOjet++ atlas-atlas-dijets-an/v-1112.6297 tarball	L	
atlas-atlas-dijets-anxiv-1112.6297-xsec000.root :: Table 19 : d2sigma/dm_{12}dy* [pb/TeV], Anti-kT R=0.4, 0.0 <y*<0.5< td=""><td></td></y*<0.5<>		
atlas-atlas-dijets-arxiv-1112.6297-xsec001.root :: Table 20 : d2sigma/dm_{12}dy* [pb/TeV], Anti-KT R=0.4, 0.5 <y*<1.0< td=""><td>1</td><td>HTML fragment will be used as the</td></y*<1.0<>	1	HTML fragment will be used as the
atlas-atlas-dijets-anxiv-1112.6297-xsec002.root :: Table 21 : d2sigma/dm_(12)dy* [pb/TeV], Anti-kT R=0.4, 1.0 <y*<1.5< td=""><td rowspan="2">analysis record</td></y*<1.5<>	analysis record	
atlas-atlas-dijets-anxiv-1112.6297-xsec003.root :: Table 22 : d2sigma/dm_(12)dy* (pb/TeV), Anti-kT R=0.4, 1.5 <y*<2.0< td=""></y*<2.0<>		
atlas-atlas-dijets-anxiv-1112.6297-xsec004.root :: Table 23 : d2sigma/dm_{12}/dy+ (pb/TeV), Anti-kT R=0.4, 2.0 < y*<2.5		
atias-atias-dijets-arg-1112.6297-xsec006.root :: Table 24 : d2sigma/dm_(12)dy* (pb/TeV), Anti-kT R=0.4, 2.5 <y*<3.0< td=""><td></td><td></td></y*<3.0<>		
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APPLGRID project

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# Top production grids





- The fastNLO top grids for the CMS measurement [arXiv:1703.01630] at NNLO released by Czakon et al [arXiv:1704.08551]. Link
  - Code is not available
  - Poor performance : slow convolution and high memory consumption
- Tables converted to full APPLgrid tables. Link
  - Disk: 2.85 MB  $\rightarrow$  1.41 MB
  - ► Memory: 6052500 B → 3003750 B
  - $\blacktriangleright$  Time: 182 ms  $\rightarrow$  126 ms

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# Current developments : MCFM v9.0

- MCFM group has released new version on 25.09.2019 [arXiv:1909.09117]
- Features: improved integration algorithm, better control of numerical accuracy, new code structure, new processes for off-shell SM and SMEFT single-top-quark production, high-pt treatment of mass effects in H+jet process, several NNLO color-singlet processes
- APPLgrid interface is off. The old one wouldn't work anyway, due to many changes in the MCFM code
- In contact with authors to re-enable the APPLgrid interface for the new versions (\*)
  - ► LO, REAL, VIRT contributions already implemented and validated
  - NNLO contribution is in progress
  - The mcmf-bridge user interface is updated
  - based on the text steering file
  - allows to fully configure the observable w/o recompiling the package
     (\*) together with Vlad Danilov (CMS-DESY)

#### Contact interactions in jet production

- NLO calculations done by Jun Gao [arXiv:1204.4773]
- Original code takes some ideas from APPLgrid and generates matrix elements tables in a special (internal) format. The convolution script allows predictions for any PDF/strong coupling/Lambda a-posteriori

- Works nicely for plotting, but quite inconvenient, for fitting purposes...
- Interface C-APPLgrid is in progress



### Summary

Precision measurements of QCD improve knowledge of PDFs and strong coupling constant and might facilitate discoveries at the LHC.

- APPLgrid is an open project, complete source code is available as HEPforge package
- A posteriori evaluation of uncertainties from renormalisation and factorisation scale variations, strong coupling measurement and PDFs error sets in a very short time
- Allows rigorous inclusion of collider data in a PDF/strong coupling fit.
- Other functionality, such as  $\sqrt{S}$  rescaling, change of initial hadrons
- A list of QCD and electroweak processes can be studied
  - Jet production studied using NLOJET++ , NNLOJET
  - Drell-Yan production via NNLOJET, MCFM, DYNNLO
  - Many other processes via MCFM , SHERPA, aMC@NLO, ContactInteractions
    - ★ W/Z/γ; W/Zγ+jet; tt, bb, cc; W+charm, any process with a basic decomposition

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# **BACK-UP**

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APPLGRID project

xFitter meeting 26/25

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