

# Fast simulations with NNLO QCD accuracy

8th International Workshop on High Precision for Hard Processes | Newcastle upon Tyne

Lucas Kunz | 20/09/2022

KARLSRUHE INSTITUTE OF TECHNOLOGY

*APPLfast*



*APPLgrid project*

**fast**NLO

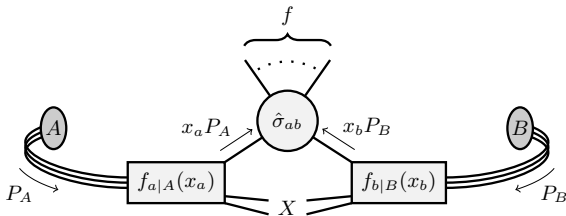


Figure by A. Huss

$$\begin{aligned}
 d\sigma_{pp \rightarrow X} = & \sum_{a,b} \int_0^1 dx_1 \int_0^1 dx_2 f_a(x_a, \alpha_s(\mu_R), \mu_F) f_b(x_b, \alpha_s(\mu_R), \mu_F) \\
 & \times d\hat{\sigma}_{ab \rightarrow X}(x_1, x_2, \alpha_s(\mu_R), \mu_R, \mu_F) + \mathcal{O}\left(\frac{\Lambda_{\text{QCD}}}{Q}\right)^p
 \end{aligned}$$

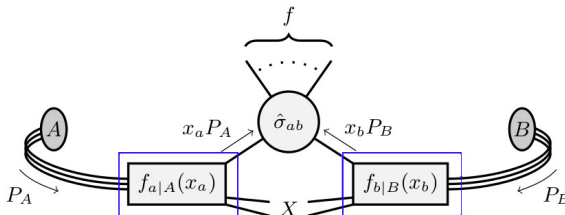


Figure by A. Huss

$$\begin{aligned}
 d\sigma_{pp \rightarrow X} = & \sum_{a,b} \int_0^1 dx_1 \int_0^1 dx_2 \, f_a(x_a, \alpha_s(\mu_R), \mu_F) f_b(x_b, \alpha_s(\mu_R), \mu_F) \\
 & \times d\hat{\sigma}_{ab \rightarrow X}(x_1, x_2, \alpha_s(\mu_R), \mu_R, \mu_F) + \mathcal{O}\left(\frac{\Lambda_{\text{QCD}}}{Q}\right)^p
 \end{aligned}$$

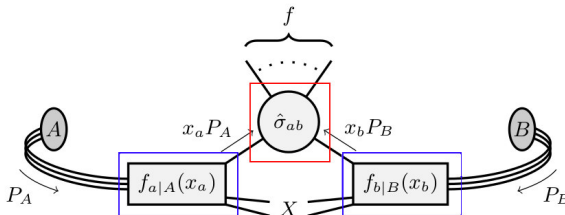


Figure by A. Huss

$$\begin{aligned}
 d\sigma_{pp \rightarrow X} = & \sum_{a,b} \int_0^1 dx_1 \int_0^1 dx_2 \quad f_a(x_a, \alpha_s(\mu_R), \mu_F) f_b(x_b, \alpha_s(\mu_R), \mu_F) \\
 & \times d\hat{\sigma}_{ab \rightarrow X}(x_1, x_2, \alpha_s(\mu_R), \mu_R, \mu_F) + \mathcal{O}\left(\frac{\Lambda_{\text{QCD}}}{Q}\right)^p
 \end{aligned}$$

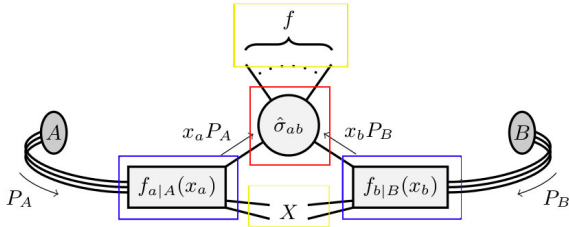
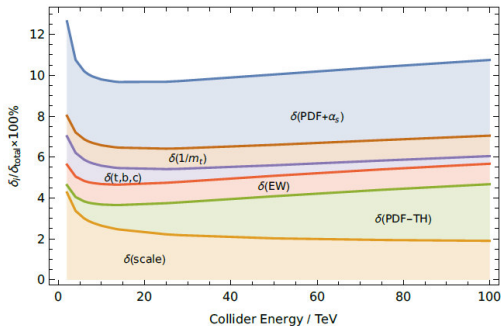


Figure by A. Huss

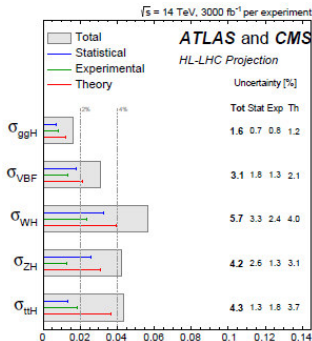
$$\begin{aligned}
 d\sigma_{pp \rightarrow X} = & \sum_{a,b} \int_0^1 dx_1 \int_0^1 dx_2 \quad f_a(x_a, \alpha_s(\mu_R), \mu_F) f_b(x_b, \alpha_s(\mu_R), \mu_F) \\
 & \times d\hat{\sigma}_{ab \rightarrow X}(x_1, x_2, \alpha_s(\mu_R), \mu_R, \mu_F) + \mathcal{O}\left(\frac{\Lambda_{\text{QCD}}}{Q}\right)^p
 \end{aligned}$$

# Motivation



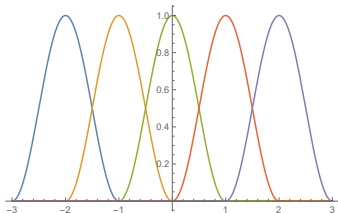
*Relative uncertainty of the Higgs boson production cross section*

*[Dulat, Lazopoulos, Mistlberger '18]*



*Higgs production uncertainty estimates for the HL-LHC*

*[HL-LHC Working Group 2 '19]*



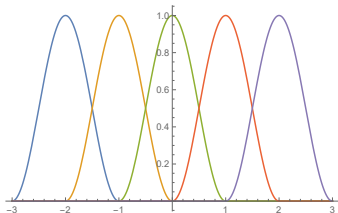
- Split interval  $I = [a, b]$  into  $N + 1$  nodes,  $a = x^{[0]}$ ,  $b = x^{[N]}$
- Partition of unity into a set of functions:
  - $1 = \sum_{i=0}^N E_i(x) \quad \forall x \in I$
  - $E_i(x^{[j]}) = 1 \quad \forall i \in \{0, \dots, N\}$

- $\Rightarrow$  Functions on the interval can be approximated:

$$f(x) \simeq \sum_{i=0}^N f^{[i]} E_i(x) \text{ where } f^{[i]} = f(x^{[i]})$$

- $\Rightarrow$  Integrals can also be approximated:

$$\int_a^b f(x)g(x) dx \simeq \sum_{i=0}^N f^{[i]} g_{[i]} \text{ with } g_{[i]} := \int_a^b E_i(x)g(x) dx$$



- Split interval  $I = [a, b]$  into  $N + 1$  nodes,  $a = x^{[0]}$ ,  $b = x^{[N]}$
- Partition of unity into a set of functions:
  - $1 = \sum_{i=0}^N E_i(x) \quad \forall x \in I$
  - $E_i(x^{[j]}) = 1 \quad \forall i \in \{0, \dots, N\}$

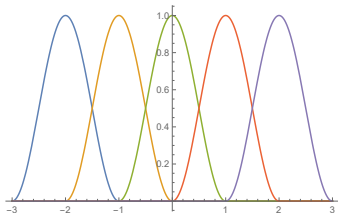
- $\Rightarrow$  Functions on the interval can be approximated:

$$f(x) \simeq \sum_{i=0}^N f^{[i]} E_i(x) \text{ where } f^{[i]} = f(x^{[i]})$$

- $\Rightarrow$  Integrals can also be approximated:

$$\int_a^b f(x)g(x) dx \simeq \sum_{i=0}^N f^{[i]} g_{[i]} \text{ with } g_{[i]} := \int_a^b E_i(x)g(x) dx$$





- Split interval  $I = [a, b]$  into  $N + 1$  nodes,  $a = x^{[0]}$ ,  $b = x^{[N]}$
- Partition of unity into a set of functions:
  - $1 = \sum_{i=0}^N E_i(x) \quad \forall x \in I$
  - $E_i(x^{[j]}) = 1 \quad \forall i \in \{0, \dots, N\}$

- $\Rightarrow$  Functions on the interval can be approximated:

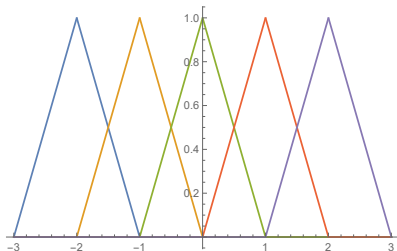
$$f(x) \simeq \sum_{i=0}^N f^{[i]} E_i(x) \text{ where } f^{[i]} = f(x^{[i]})$$

- $\Rightarrow$  Integrals can also be approximated:

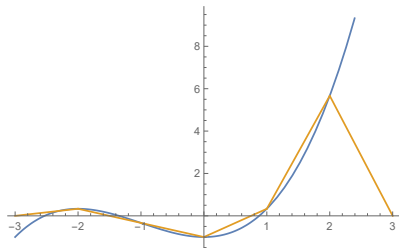
$$\int_a^b f(x)g(x) dx \simeq \sum_{i=0}^N f^{[i]} g_{[i]} \text{ with } g_{[i]} := \int_a^b E_i(x)g(x) dx$$

Example:  $f(x) = \frac{1}{3}x^3 + x^2 - 1$  on the Interval  $I = [-2, 2]$

Five nodes  $\{-2, -1, 0, 1, 2\}$

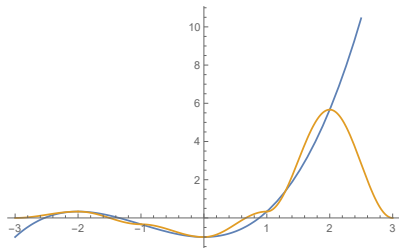
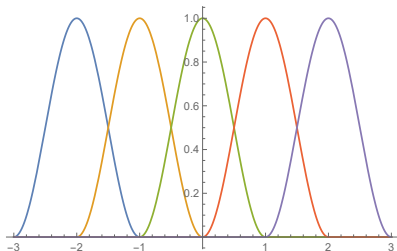


$\Rightarrow$



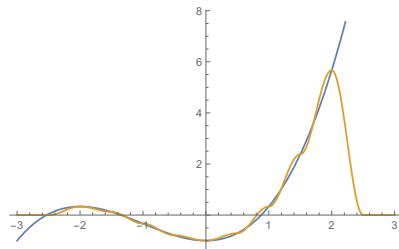
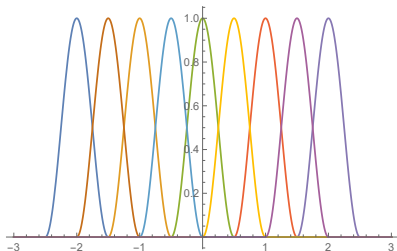
Example:  $f(x) = \frac{1}{3} x^3 + x^2 - 1$  on the Interval  $I = [-2, 2]$

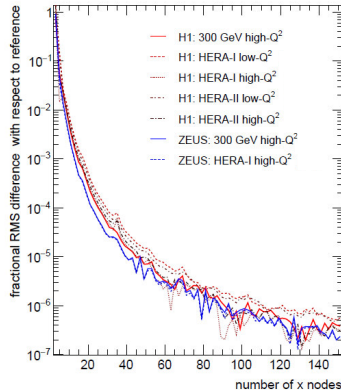
Five nodes  $\{-2, -1, 0, 1, 2\}$



Example:  $f(x) = \frac{1}{3}x^3 + x^2 - 1$  on the Interval  $I = [-2, 2]$

Nine nodes  $\{-2, -1.5, \dots, 1.5, 2\}$





*Fractional root mean square difference between interpolation and reference*  
*[Britzger, Gehrmann, Huss, Rabbertz, et al. '19]*

$$d\hat{\sigma}_{ab \rightarrow X}(x, \alpha_s, \mu) = \sum_k \left( \frac{\alpha_s(\mu_R)}{2\pi} \right)^{k+r} d\hat{\sigma}_{ab \rightarrow X}^{(k)}(x, \alpha_s, \mu)$$

Evaluation with Monte Carlo event generator:

- Fixed-order ( $k = 0, 1, \dots$ ) parton level calculations
- Phase-space samples  $(x_m, \Phi_m)$  with weights  $w_{ab \rightarrow X, m}^{(k)}$

$$\begin{aligned} \Rightarrow \sigma_{pp \rightarrow X}(x, \alpha_s, \mu) &= \sum_{a,b} \sum_k \sum_{m=1}^{M_p} \left( \frac{\alpha_s(\mu_{R,m})}{2\pi} \right)^{k+r} \hat{\sigma}_{ab \rightarrow X, m}^{(k)} \\ &\quad \times w_{ab \rightarrow X, m}^{(k)} f_a(x_{a,m}, \mu_{F,m}) f_b(x_{b,m}, \mu_{F,m}) \end{aligned}$$

For pp collisions: 4 functions  $E_i(x_a)$ ,  $E_j(x_b)$ ,  $E_v(\mu_R)$ ,  $E_w(\mu_F)$

$$\Rightarrow \sigma_{pp \rightarrow X}(X, \alpha_s, \mu) = \sum_{i,j,v,w=0}^N \sum_{a,b} \sum_k \left( \frac{\alpha_s^{[v]}}{2\pi} \right)^{k+r} f_a^{[i,w]} f_b^{[j,w]} \times \hat{\sigma}_{ab \rightarrow X}^{(k)}[i,j,v,w]$$

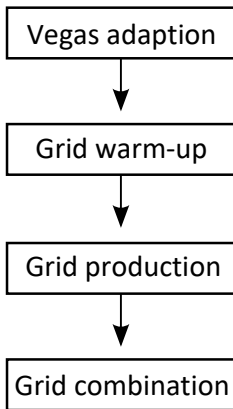
with

$$\hat{\sigma}_{ab \rightarrow X}^{(k)}[i,j,v,w] := \sum_{m=1}^{M_p} E_i(x_{a,m}) E_j(x_{b,m}) E_v(\mu_{R,m}) E_w(\mu_{F,m}) \times w_{ab \rightarrow X, m}^{(k)} \hat{\sigma}_{ab \rightarrow X, m}^{(k)}$$

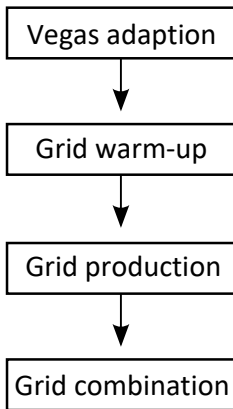
- NNLOJET: fixed order Monte Carlo calculations
- fastNLO/APPLgrid: grid libraries
- APPLfast: interface connecting the two sides



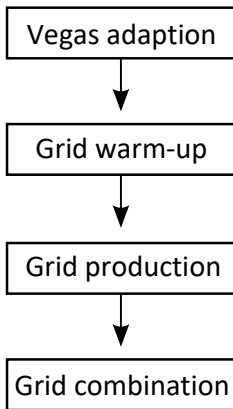




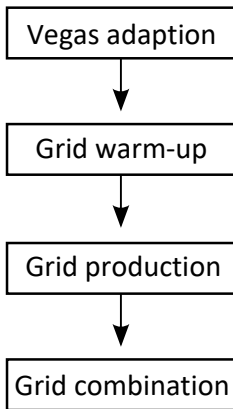
- generate optimised Vegas phase-space grid
- optimise the limits for  $x$  and  $\mu$  (experimental fiducial cuts)
- grids filled with the weights generated from a full NNLOJET run
- grids from individual jobs are combined into final master grid



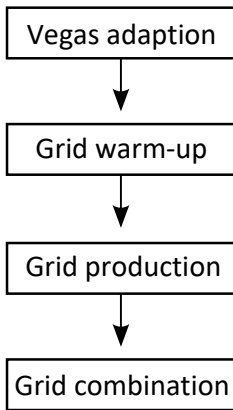
- generate optimised Vegas phase-space grid
- optimise the limits for  $x$  and  $\mu$  (experimental fiducial cuts)
- grids filled with the weights generated from a full NNLOJET run
- grids from individual jobs are combined into final master grid



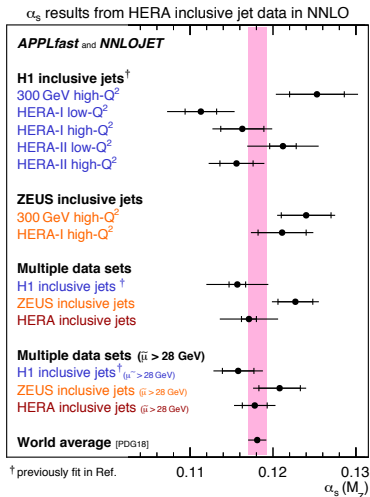
- generate optimised Vegas phase-space grid
- optimise the limits for  $x$  and  $\mu$  (experimental fiducial cuts)
- grids filled with the weights generated from a full NNLOJET run
- grids from individual jobs are combined into final master grid



- generate optimised Vegas phase-space grid
- optimise the limits for  $x$  and  $\mu$  (experimental fiducial cuts)
- grids filled with the weights generated from a full NNLOJET run
- grids from individual jobs are combined into final master grid

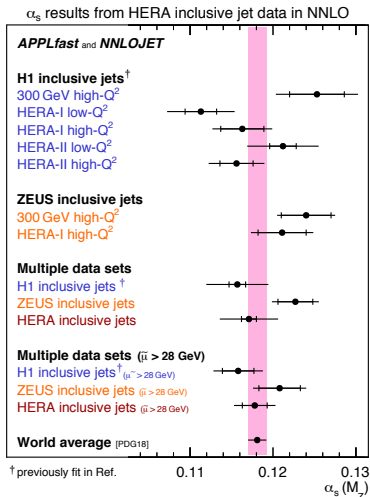


- generate optimised Vegas phase-space grid
- optimise the limits for  $x$  and  $\mu$  (experimental fiducial cuts)
- grids filled with the weights generated from a full NNLOJET run
- grids from individual jobs are combined into final master grid



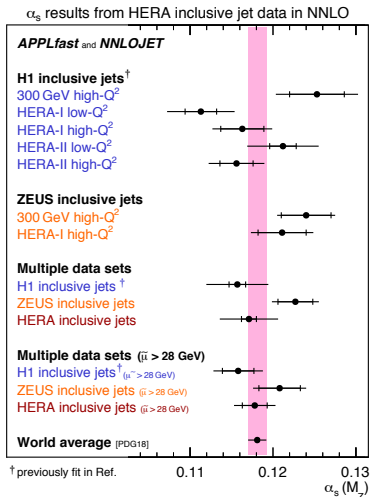
## Use cases:

- observable calculations
  - PDF fitting
  - determination of the strong coupling constant
- [H1 collaboration '17]
- [Britzger, Gehrmann, Huss, Rabbertz, et al. '19]
- [Britzger, Gehrmann, Huss, Rabbertz, et al. '22]



## Use cases:

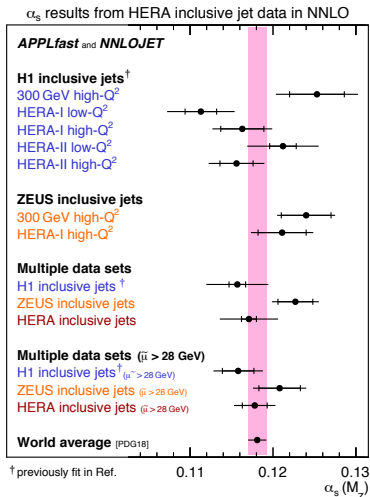
- observable calculations
  - PDF fitting
  - determination of the strong coupling constant
- [H1 collaboration '17]  
[Britzger, Gehrmann, Huss, Rabbertz, et al. '19]  
[Britzger, Gehrmann, Huss, Rabbertz, et al. '22]



## Use cases:

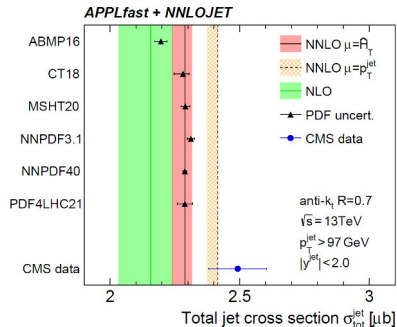
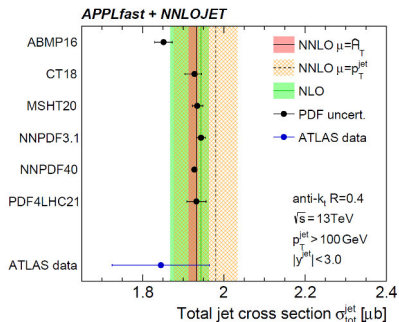
- observable calculations
  - PDF fitting
  - determination of the strong coupling constant
- [H1 collaboration '17]  
[Britzger, Gehrmann, Huss, Rabbertz, et al. '19]  
[Britzger, Gehrmann, Huss, Rabbertz, et al. '22]





## Use cases:

- observable calculations
  - PDF fitting
  - determination of the strong coupling constant
- [H1 collaboration '17]  
 [Britzger, Gehrmann, Huss, Rabbertz, et al. '19]  
 [Britzger, Gehrmann, Huss, Rabbertz, et al. '22]



Comparison of the total jet cross section using different PDFs  
 [Britzger, Gehrmann, Huss, Rabbertz, et al. '22]

- Interface adapted to use modules 2 of NNLOJET
  - better colour sampling
  - full colour dijet code
  - more flexible decomposition of logarithmic scale coefficients
- Validation at NNLO in progress
- Runtime comparison at NLO (in minutes, Drell-Yan, 1000000 events):

| setup     | warmup (LO/R/V) |       |       | production (LO/R/V) |      |       |
|-----------|-----------------|-------|-------|---------------------|------|-------|
| modules 1 | 18.75           | 20.32 | 35.53 | 2.41                | 8.99 | 10.62 |
| modules 2 | 3.48            | 5.59  | 17.49 | 0.776               | 1.70 | 6.85  |

- finalize validation of NNLO code
  - produce grids for jet+X and di-jet processes at the LHC
  - extract value of  $\alpha_s(M_Z)$  from LHC data
  - reproduce results in [\[Britzger, Gehrmann, Huss, Rabbertz, et al. '22\]](#)
- optimize workflow and runtime
- calculate di-jet differential distributions at full colour
- provide setup for further developments and calculations

**Thank you for your attention!**

$$\sigma_{pp \rightarrow X}(X, \alpha_s, \mu) = \sum_{i,j,v,w=0}^N \sum_{a,b} \sum_k \left( \frac{\alpha_s^{[v]}}{2\pi} \right)^{k+r} f_a^{[i,w]} f_b^{[j,w]} \hat{\sigma}_{ab \rightarrow X}^{(k)}[i,j,v,w]$$

$$d\hat{\sigma}_{ab \rightarrow X}^{(k)}[i,j,v,w](\mu_R^2, \mu_F^2) = \sum_{\alpha+\beta \leq k} d\hat{\sigma}_{ab \rightarrow X}^{(k|\alpha,\beta)}[i,j,v,w] \ln^\alpha \left( \frac{\mu_R^2}{\mu_0^2} \right) \ln^\beta \left( \frac{\mu_F^2}{\mu_0^2} \right)$$

$$\hat{\sigma}_{ab \rightarrow X}^{(k|\alpha,\beta)}[i,j,v,w] = \sum_{m=1}^{M_p} E_i(x_{a,m}) E_j(x_{b,m}) E_v(\mu_{R,m}) E_w(\mu_{F,m}) w_{ab \rightarrow X,m}^{(k)} \hat{\sigma}_{ab \rightarrow X,m}^{(k|\alpha,\beta)}$$