New simpler methods of matching NLO corrections with parton shower Monte Carlo

S. JADACH

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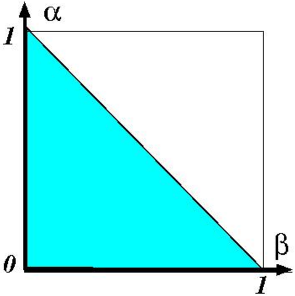
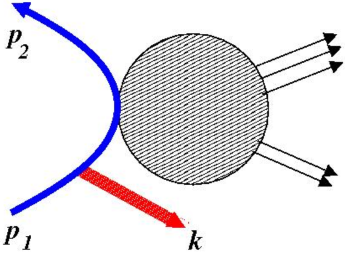
NLO corrections to hard process, KrkNLO method

1. Methodology of the KrkNLO for DY process was defined in Ustron 2011 Proc., but without numerical test:
   Acta Phys.Polon. B42 (2011) 2433 , [arXiv:1111.5368]
2. Numerical validation on top of Double-CMC toy model PS MC in:
   Acta Phys.Polon. B43 (2012) 2067 , [arXiv:1209.4291]
3. Complete theoretical discussion of the KrkNLO scheme, introducing PDFs in the MC factorization scheme in:
   Phys.Rev. D87 (2013) 3, 034029 , [arXiv:1103.5015],
   implementation still using not so realistic Double-CMC PS.
4. First realistic implementation of top of SHERPA and HERWIG in *JHEP 1510 (2015) 052* [arXiv:1503.06849], including also comparisons of KrkNLO numerical results with NLO and NNLO calculat(fixed order), MC@NLO and POWHEG, all that for Drell-Yan process.
5. NEW in this presentation: (i) Mature definition of PDFs in the MC factorization scheme (ii) more on universality, (iii) application to Higgs production process.

Sudakov variables in DY

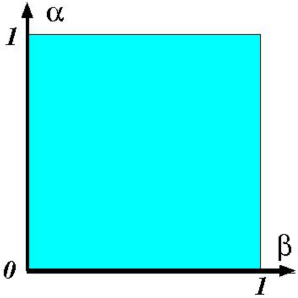


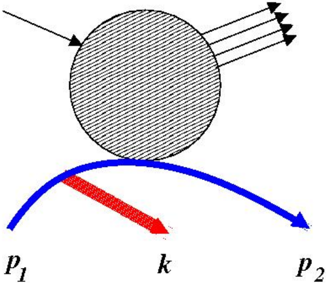


$$\alpha = \frac{(kp_1)}{(p_1 p_2)}, \quad \beta = \frac{(kp_2)}{(p_1 p_2)},$$

$$\alpha + \beta \leq 1, \quad \alpha \geq 0, \ \beta \geq 0.$$

Sudakov variables in DIS





$$\alpha = \frac{(kp_1)}{(p_1p_2)+(kp_1)}, \quad \beta = \frac{(kp_2)}{(p_1p_2)+(kp_1)},$$

$$\max(\alpha,\beta) \le 1, \quad \alpha \ge 0,\ \beta \ge 0.$$

Recipe of the KrkNLO method is unbelievably simple:

Spin zero Higgs production

Take event generated by the LO parton shower MC as is and apply simple positive well behaved weight:

- $g + g \longrightarrow H, H + g$:

$$W_{gg}^{\rm MC}(\alpha,\beta) = \frac{1+z^4+\alpha^4+\beta^4}{1+z^4+(1-z)^4}(1+\Delta_{VS}^{\rm MC}),$$

$$\Delta_{VS}^{\rm MC} = \frac{\alpha_s}{2\pi}\,2C_A\left[\frac{473}{72}+\frac{2\pi^2}{3}-\frac{T_f}{C_A}\frac{59}{36}\right].$$

- $g + q \longrightarrow H + q$:

$$W_{gq}^{\rm MC}(\alpha,\beta) = \frac{1+\beta^2}{1+(1-z)^2} \quad \leq 1,$$

The above recipe is dramatically simpler than POWHEG or MC&NLO. However, several nontrivial conditions has to be met before it works.
Most important are:
(1) the use of PDFs in the physical MC factorization scheme,
(2) certain minimum quality of the PS MC, see next slides.

Recipe of the KrkNLO method is extremely simple:

$pp \to Z/\gamma^*$, DY

Take event generated by the LO parton shower MC as is and apply simple positive well behaved weight:

- $q + \bar{q} \longrightarrow Z, Z + g$

$$W^{\rm MC}_{q\bar{q}}(\alpha,\beta) = \left\langle \frac{|\mathcal{M}^{\rm NLO}_{q\bar{q}\to Zg}|^2}{|\mathcal{M}^{\rm MC}_{q\bar{q}\to Zg}|^2} \right\rangle_{\rm Z\ decay} = \left(1 - \frac{2\alpha\beta}{1+z^2}\right)(1+\Delta^{\rm MC}_{VS}),$$

$$\Delta^{\rm MC}_{VS} = \frac{\alpha_s}{2\pi}\left(\frac{4\pi^2}{3} + \frac{1}{2}\right).$$

- $q + g \longrightarrow Z + q$:

$$W^{\rm MC}_{qg}(\alpha,\beta) = \left\langle \frac{|\mathcal{M}^{\rm NLO}_{qg\to Zq}|^2}{|\mathcal{M}^{\rm MC}_{qg\to Zq}|^2} \right\rangle_{\rm Z\ deday} = 1 + \frac{\alpha(\alpha+2z)}{z^2+(1-z)^2}.$$

Without averaging over Z decay MC weight is also quite simple, see next slide.

Immediate question: Which α, β? Which parton?
Answer: of the parton with maximum kT

- For PSMC with kT-ordering, the 1-st parton in the backward evolution.
- For angular ordering parton with maximum kT to be found in MC event.
- Alternatively, one may use formula with "democratic" sum over all gluons. An example of multiple gluon emission in DY:

$$d\sigma_n^{\rm NLO} = \Big(1 + \Delta_{VS} + \sum_{i=1}^{n} W_{q\bar q}^{[1]}(\alpha_i,\beta_i)\Big)\, d\sigma_n^{\rm LO},$$

$$W_{q\bar q}^{[1]} = \frac{d^5\bar\beta_{q\bar q}}{d^5\sigma_{q\bar q}^{\rm LO}} = \frac{d^5\sigma_{q\bar q}^{\rm NLO} - d^5\sigma_{q\bar q}^{\rm LO}}{d^5\sigma_{q\bar q}^{\rm LO}}, \qquad \Delta_{VS}^{q\bar q} = \frac{\alpha_s}{2\pi} C_F \left[\frac{4}{3}\pi^2 - \frac{5}{2}\right],$$

$$d^5\sigma_{q\bar q}^{NLO}(\alpha,\beta,\Omega) = \frac{C_F\alpha_s}{\pi}\, \frac{d\alpha\, d\beta}{\alpha\beta}\, \frac{d\varphi}{2\pi}\, d\Omega \left[\frac{d\sigma_0(\hat s,\theta_F)}{d\Omega}\, \frac{(1-\beta)^2}{2} + \frac{d\sigma_0(\hat s,\theta_B)}{d\Omega}\, \frac{(1-\alpha)^2}{2}\right],$$

$$d^5\sigma_{q\bar q}^{\rm LO}(\alpha,\beta,\Omega) = d^5\sigma_{q\bar q}^{F} + d^5\sigma_{q\bar q}^{B} = \frac{C_F\alpha_s}{\pi}\, \frac{d\alpha\, d\beta}{\alpha\beta}\, \frac{d\varphi}{2\pi} d\Omega\, \frac{1 + (1-\alpha-\beta)^2}{2}\, \frac{d\sigma_0}{d\Omega}(\hat s,\hat\theta),$$

- Sudakov suppression of soft limit exploited as in POWHEG, but no need of truncated shower for angular ordering.

Conditions for KrkNLO methodology to work

and other issues to be clarified

- **PDFs in MC factorization scheme – an absolute must!**
- **LO PSMC reproduces precisely all collinear and soft singularities of the NLO** ***(nontrivial for LO processes with*** ≥ 3 ***coloured legs)*** **and covers the entire NLO phase space**
- **The question of universality of the MC factorization scheme. Does it work for** ≥ 3 **coloured emitters at LO?**

Definition of LO PDFs in MC factorization scheme

in terms of PDFs in $\overline{MS}$ scheme

$$\begin{bmatrix} q(x,Q^2) \\ \bar{q}(x,Q^2) \\ G(x,Q^2) \end{bmatrix}_{\rm MC} = \begin{bmatrix} q \\ \bar{q} \\ G \end{bmatrix}_{\overline{MS}} + \int dz dy \begin{bmatrix} K^{\rm MC}_{qq}(z) & 0 & K^{\rm MC}_{qG}(z) \\ 0 & K^{\rm MC}_{\bar{q}\bar{q}}(z) & K^{\rm MC}_{\bar{q}G}(z) \\ K^{\rm MC}_{Gq}(z) & K^{\rm MC}_{G\bar{q}}(z) & K^{\rm MC}_{GG}(z) \end{bmatrix} \begin{bmatrix} q(y,Q^2) \\ \bar{q}(y,Q^2) \\ G(y,Q^2) \end{bmatrix}_{\overline{MS}} \delta(x-yz)$$

where

$$K^{\rm MC}_{Gq}(z) = \frac{\alpha_S}{2\pi}\, C_F \left\{ \frac{1+(1-z)^2}{z} \ln\frac{(1-z)^2}{z} + z \right\},$$

$$K^{\rm MC}_{GG}(z) = \frac{\alpha_S}{2\pi}\, C_A \left\{ 4\left[\frac{\ln(1-z)}{1-z}\right]_+ + 2\left[\frac{1}{z} - 2 + z(1-z)\right] \ln\frac{(1-z)^2}{z} - 2\frac{\ln z}{1-z} - \delta(1-z)\left(\frac{\pi^2}{3} + \frac{341}{72} - \frac{59}{36}\frac{T_f}{C_A}\right),\right.$$

$$K^{\rm MC}_{qq}(z) = \frac{\alpha_S}{2\pi}\, C_F \left\{ 4\left[\frac{\ln(1-z)}{1-z}\right]_+ - (1+z)\ln\frac{(1-z)^2}{z} - 2\frac{\ln z}{1-z} + 1 - z - \delta(1-z)\left(\frac{\pi^2}{3} + \frac{17}{4}\right) \right\},$$

$$K^{\rm MC}_{qG}(z) = \frac{\alpha_S}{2\pi}\, T_R \left\{ \left[z^2 + (1-z)^2\right] \ln\frac{(1-z)^2}{z} + 2z(1-z) \right\}.$$

All virtual parts $\sim \delta(1-z)$ adjusted using momentum sum rules.
Direct fitting PDFs to DIS data requires MC-scheme coeff. functions, see below...
Q^2 evolution governed by LO kernels.

Fitting MC-scheme PDFs (LO) directly to DIS data

requires MC-scheme NLO coefficient functions

$$C^{\rm MC}_{2,qq}(z) = \frac{\alpha_s}{2\pi}\, C_F \left\{ \left[-\frac{1+z^2}{1-z}\ln(1-z) - \frac{3}{2}\frac{1}{1-z} + 3z + 2 \right]_+ + \frac{3}{2}\,\delta(1-z) \right\},$$

instead of $C^{\overline{MS}}_{2,qq}(z) = \frac{\alpha_s}{2\pi}\, C_F \left[\frac{1+z^2}{1-z}\ln\frac{1-z}{z} - \frac{3}{2}\frac{1}{1-z} + 2z + 3 \right]_+$ and

$$C^{\rm MC}_{2,qG}(z) = \frac{\alpha_s}{2\pi}\, T_R \left\{ -\left[z^2 + (1-z)^2\right]\ln(1-z) + 6z(1-z) - 1 \right\}$$

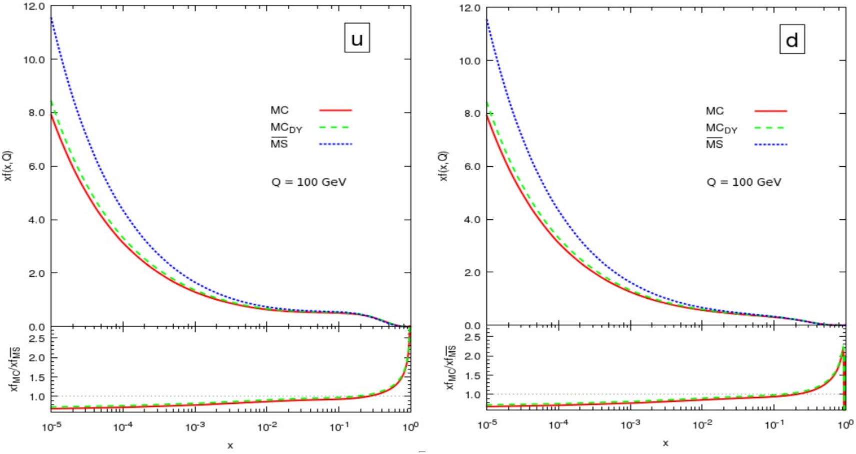
instead of $C^{\overline{MS}}_{2,qG}(z) = \frac{\alpha_s}{2\pi}\, T_R \left\{ \left[z^2 + (1-z)^2\right]\ln\frac{1-z}{z} + 8z(1-z) - 1 \right\}$.

MC factorization scheme

- What is the purpose of MC fact.scheme?
  – It is defined such that $\Sigma(z)\delta(k_T)$ terms due to emission from initial partons disappear completely from exclusive NLO corrections, even before PSMC gets involved!.
- Why the above is vital in the KrkNLO scheme?
  – Without eliminating them it is not possible to include NLO correction with a multipicative MC weights on top of the PSMC distributions.
- How to determine elements of the transition matrix $K^{\rm MC}_{ab}$?
  – Obtained from inspecting NLO corrs. to two processes with quarks and gluons in the LO hard process: Z and Higgs boson production.
- Will the same PDFs eliminate $\sim \delta(k_T)$ terms for other processes?
  It was shown already in *Phys.Rev. D87 (2013)* that for DIS it works.
- For any other process may work,
  provided PSMC distribution obeys certain extra conditions.
  This is a question about *universality* of the MC fact.scheme.

MC factorization scheme

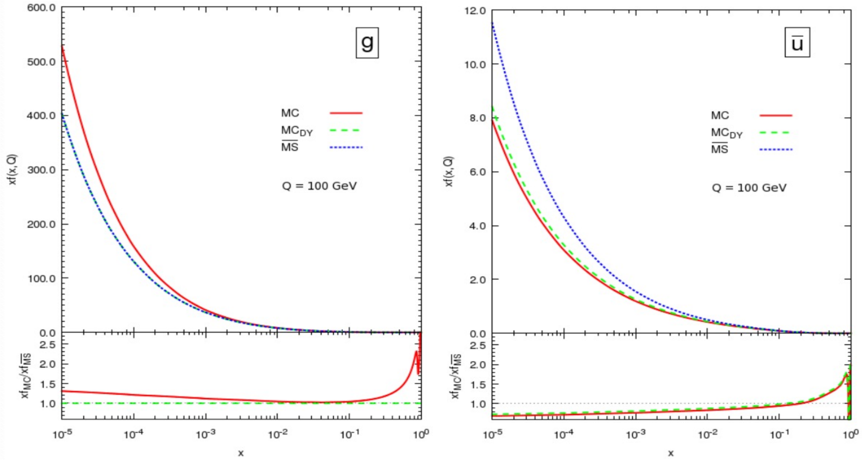
Numerical examples of PDFs in the MC scheme



- Change with respect to $\overline{MS}$ PDFs is noticeable.
- Version labeled MC is complete MC scheme.
- Version MC$_{DY}$ neglects certain $\mathcal{O}(\alpha_s^2)$ terms, limited to DY process.

MC factorization scheme

Numerical examples of PDFs in the MC scheme

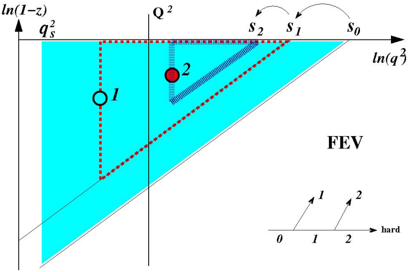


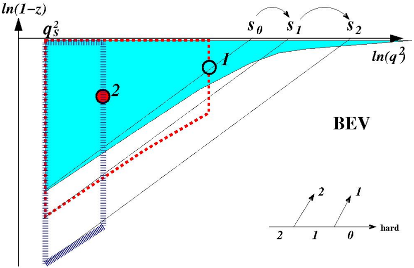
- Change with respect to $\overline{MS}$ PDFs is noticeable.
- Version labeled MC is complete MC scheme.
- Version MC_{DY} neglects certain $\mathcal{O}(\alpha_s^2)$ terms, limited to DY process.

Parton shower MC related issues:

Full coverage of the hard gluon phase space by LO PSMC is essential for KrkNLO!

Phase space limits in forward (FEV) and backward (BEV) evolution for up to 2 emissions. BEV looks more complicated:





Luckily in modern LO PS MCs like Sherpa and Herwig full phase space coverage is implemented, in spite of the above complication, thanks to combination of veto and BEV algorithms.

See *JHEP 1510 (2015) 052* [arXiv:1503.06849] for more details.

Another Parton shower MC related issue:

Compatibility of forward (FEV) and backward (BEV) distribs. up to NLO

Forward evol.

$$\sigma^{\rm LO}_{\rm MC} = \int dx_F dx_B d\Omega \sum_{n_F=0}^{\infty} \sum_{n_B=0}^{\infty} \int d\sigma^{\rm LO}_{n_F n_B},$$

$$d\sigma^{\rm LO}_{n_F n_B} = \prod_{i=1}^{n_F} \prod_{j=1}^{n_B} \Big\{ \int d^3\rho_i^F \theta_{q_{i-1}^2 > q_i^2 > q_s^2}\, e^{-S_F(q_{i-1}^2, q_i^2)} \Big\} \Big\{ \int d^3\rho_j^B \theta_{q_{j-1}^2 > q_j^2 > q_s^2}\, e^{-S_B(q_{j-1}^2, q_j^2)} \Big\}$$
$$\times\, e^{-S_F(q_{n_F}^2, q_s^2)} e^{-S_B(q_{n_B}^2, q_s^2)} \frac{d\sigma}{d\Omega}(s x_F x_B, \hat\theta) \frac{1}{Z_{n_F}} D^F_{\rm MC}\Big(q_s^2, \frac{x_F}{Z^F_{n_F}}\Big)\, \frac{1}{Z_{n_B}} D^B_{\rm MC}\Big(q_s^2, \frac{x_B}{Z^B_{n_B}}\Big),$$

$$d^3\rho_i^F = d^3\rho_i^F(s_{ij}) = \frac{d\tilde\beta_i d\tilde\alpha_i}{\tilde\beta_i(\tilde\alpha_i + \tilde\beta_i)} \frac{d\phi_i}{2\pi}\; \bar{\mathcal{P}}(1 - \tilde\alpha_i - \tilde\beta_i)\, \theta_{\tilde\alpha_i > 0}\, \theta_{\tilde\alpha_i + \tilde\beta_i < 1}$$
$$= \frac{dq_i^2 dz_i}{q_i^2} \frac{d\phi_i}{2\pi} \theta_{(1-z_i)^2 s_{ij} > q_i^2} \mathcal{P}(z_i) = \frac{dq_i^2}{q_i^2} \frac{d\phi_i}{2\pi} dz_i \frac{\bar{\mathcal{P}}(z_i)}{1 - z_i} \theta_{(1-z_i)^2 s_{ij} > q_i^2},$$

$$S_F(q_b^2, q_a^2) = S_F(s_{ij}|q_b^2, q_a^2) \equiv \int_{q_a^2 < q_i^2 < q_b^2} d^3\rho_i^F(s_{ij}),$$

Backward evolution

$$d\sigma^{\rm LO}_{n_F n_B} = \frac{d\sigma}{d\Omega}(s x_F x_B, \hat\theta) \prod_{i=1}^{n_F} \Big\{ d^3\omega_i^F\; \theta_{q_{i-1}^2 > q_i^2} \Big\} \prod_{j=1}^{n_B} \Big\{ d^3\omega_j^B\; \theta_{q_{j-1}^2 > q_j^2} \Big\}$$
$$\times\, e^{-\Delta_F(x^F_{n_F}|q^2_{n_F}, q_s^2)} e^{-\Delta_B(x^B_{n_B}|q^2_{n_B}, q_s^2)} D^F(\hat s, x_F)\, D^B(\hat s, x_B)\, dx_F dx_B d\Omega,$$
$$x_i^F = x_F/Z_i^F,\; x_j^B = x_B/Z_j^B,\; \hat s = s x_F x_B,$$

$$d^3\omega_i^H = \frac{dq_i^2 dz_i}{q_i^2} \frac{d\phi_i}{2\pi} \mathbb{K}_{\rm MC}(x_{i-1}|z_i, q_i^2)\, e^{-\Delta_{\rm MC}(x_{i-1}|q_i^2, q_{i-1}^2)},$$

$$\mathbb{K}_{\rm MC}(x^*|z, q^2) \equiv \mathcal{P}(z_i)\, \theta_{(1-z)^2 s x^*/z > q^2}\, \frac{\overline{D}_{\rm MC}(s x^*/z | q^2, x^*/z)}{\overline{D}_{\rm MC}(s x^* | q^2, x^*)},$$

$$\Delta_{\rm MC}(x^*|q_{j-1}^2, q_j^2) \equiv \int_{q_j^2}^{q_{j-1}^2} \frac{dq^2}{q^2} \int_{x^*}^{1} \frac{dz}{z} \mathbb{K}_{\rm MC}(x^*|z, q^2),$$

Formal algebraic proof of NLO-compatibility between FEV and BEV is based on 2 elements:

1. Multiple use of identity eliminating/introducing BEV form-factor and ratios of PDFs:

$$e^{-S_{\rm MC}(\hat s|q_b^2, q_a^2)} = e^{-\Delta_{\rm MC}(x|q_b^2, q_a^2)} \frac{\overline{D}_{\rm MC}(\hat s|q_b^2, x)}{\overline{D}_{\rm MC}(\hat s|q_a^2, x)}.$$

2. And introduction of auxiliary PDFs with its own evolution equation $\bar D(Q^2, x)$, for which equality between FEV and BEV ditribs. holds *exactly*.

Final elimination of $\bar D(Q^2, x)$ provides also precise definition of PDFs in MC factoriz. scheme.

See *JHEP 1510 (2015) 052* [arXiv:1503.06849] for more details.

Universality of the KrkNLO method

Preliminary study provides positive answer (unpublished)

- Process-wise it was checked that KrkNLO method works, with **the same PDFs** in the MC factorization scheme, for DY ($q\bar{q} \to Z$) Higgs ($GG \to H$) and DIS ($eq \to eq$).
- Preliminary study within Catani-Seymour (CS) subtraction scheme shows that the same is true for any other process (any number of colored legs) provided that:
  1. Distribution from LO PS MC agree (for initial partons) with CS soft-collinear counterterms (SCC) up to NLO,
  2. CS soft-collinear counterterms are slightly redefined for “dipoles” with one initial and one final parton:
- Luckily, distributions of PS MC like modern versions of Herwig, Sherpa (Pythia?) are identical with “CS dipoles” for simple processes – this may be more problematic for more coloured legs...

Universality of the KrkNLO method

Collinear remnant in Catani Seymour scheme
from Frixione, Nason, Oleari 2007 paper

The collinear remnant is given by

$$\mathcal{G}_{\oplus}^{f_\oplus f_\ominus}(z) = \frac{\alpha_S}{2\pi} \sum_{f'_\oplus} \Bigg\{ \left[\overline{K}^{f_\oplus f'_\oplus}(z) - K_{\text{F.S.}}^{f_\oplus f'_\oplus}(z) \right] \mathcal{B}^{f'_\oplus f_\ominus}(z)$$

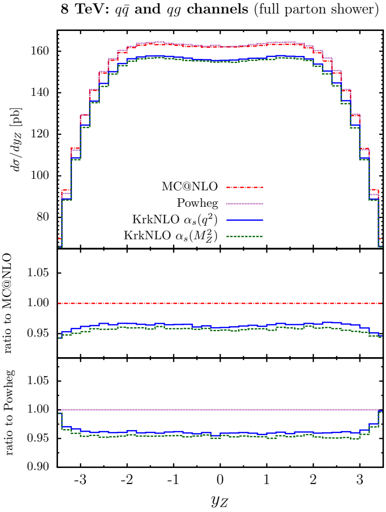
$$- \delta^{f_\oplus f'_\oplus} \sum_{i=1}^{n} \frac{\gamma_{f_i}}{C_{f_i}} \left[\left(\frac{1}{1-z} \right)_+ + \delta(1-z) \right] \mathcal{B}_{i\oplus}^{f'_\oplus f_\ominus}(z) + \frac{1}{C_{f'_\oplus}} \tilde{K}^{f_\oplus f'_\oplus}(z)\, \mathcal{B}_{\ominus\oplus}^{f'_\oplus f_\ominus}(z)$$

$$- P^{f_\oplus f'_\oplus}(z) \frac{1}{C_{f'_\oplus}} \sum_{\substack{i \in \mathcal{I} \\ i \neq \oplus}} \mathcal{B}_{i\oplus}^{f'_\oplus f_\ominus}(z) \log \frac{\mu_F^2}{2\, z\, k_\oplus \cdot k_\ominus} \Bigg\}, \tag{2.108}$$

Numerical results

DY: Comparison of the rapidity distribution

between two versions of KrkNLO and MC@NLO or POWHEG.

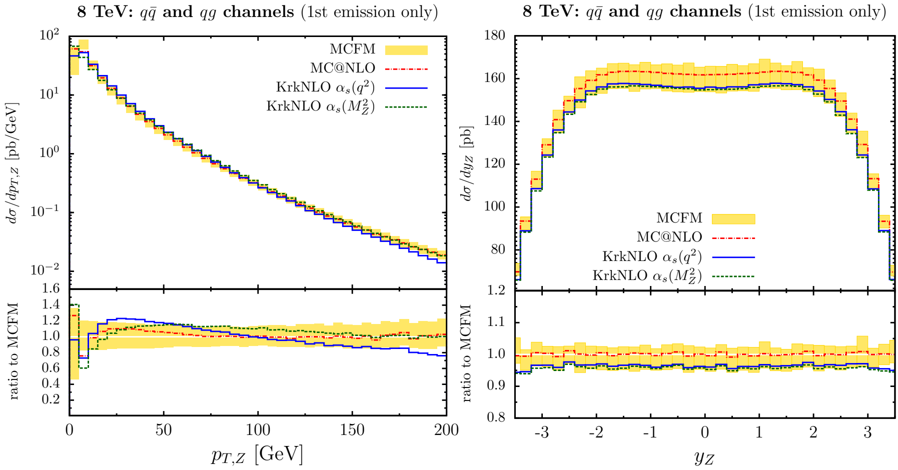


	$\sigma_{\rm tot}^{q\bar{q}+qg}$ [pb]
MCFM	1086.5 ± 0.1
MC@NLO	1086.5 ± 0.1
POWHEG	1084.2 ± 0.6
KrkNLO $\alpha_s(q^2)$	1045.4 ± 0.1
KrkNLO $\alpha_s(M_Z^2)$	1039.0 ± 0.1

Differences in rapidity distr. normalization the same as in table of total xsect.

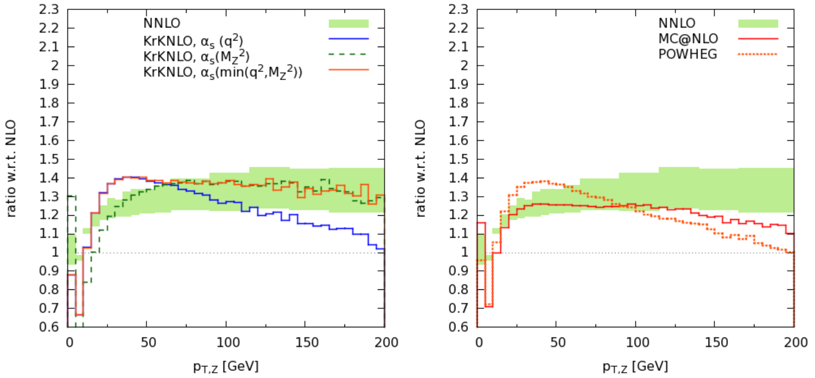
DY: Transverse momentum and rapidity distributions

from MCFM, MC@NLO and two versions of KrkNLO.



- Factorization and renormalization scale varied by 2 and 1/2 (independently).
- 10-20% differences well within uncertainty band typical for NLO.

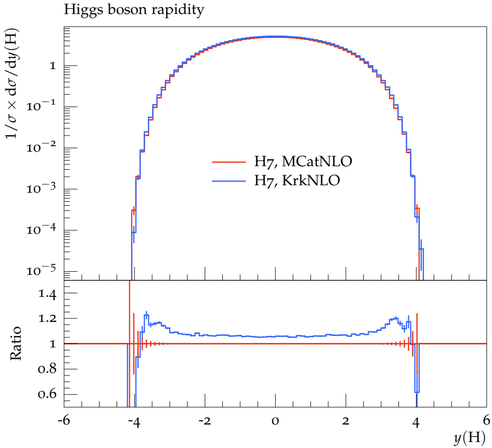
DY: Good agreement of KrkNLO with NNLO fixed order



- The Z-boson transverse-momentum distributions from KrkNLO compared with the fixed-order NNLO result from the DYNNLO (left).
- Similar comparisons for POWHEG and MCatNLO are also shown (right).
- All distributions are divided by the NLO results from MCFM.
- KrkNLO closer to NNLO than POWHEG and MCatNLO.

NEW! $pp \to H$: rapidity distrib. PRELIMINARY!

KrkNLO on top of Herwig 7 compared with MC@NLO

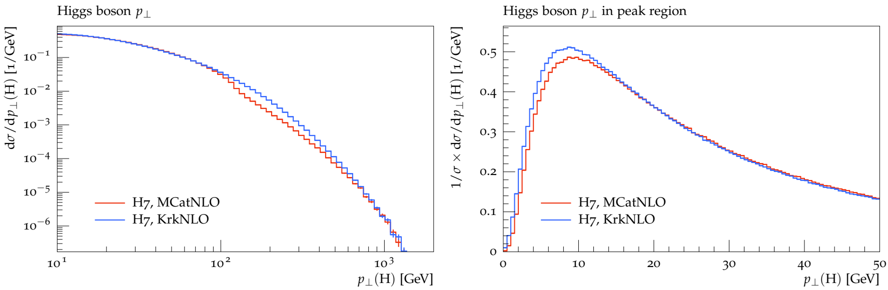


	$\sigma_{tot}[pb]$
MC@NLO	1.88 ± 0.02
KrkNLO	2.00 ± 0.02

- $\leq$ 20% differences, well within uncertainty typical for NLO.

NEW! $pp \to H$: Transverse momentum distrib. PRELIMINARY!

KrkNLO on top of Herwig 7 compared with MC@NLO



- $\leq$ 20% differences for $p_T \leq$ 100GeV, well within uncertainty typical for NLO and
- $\sim$ 200% differences for higher k_T, also well known in comparisons between POWHEG and MCatNLO for this process.

Outlook

- **KrkNLO is a simple scenario for NLO-corrected PSMC – alternative to MC@NLO or POWHEG.**
- Potential gains from new QCD methods are:
  – reducing h.o. QCD uncertainties ?
  – easier implementation of NLO and possibly NNLO corrections to hard process?
- Next applications: high quality QCD+EW+QED MC with hard process like $W/Z/H$ boson production at high luminosity LHC.
- Other fronts: Parton shower MC implementing complete NLO DGLAP in the ladders in exclusive way is shown to be possible... see Appendix.
- Longer term: N+NLO: NLO ladder + NNLO hard process.

APPENDIX

Most advanced front: NLO corrections to PS MC

- Even simpler and faster scheme of NLO-correcting PS MC (single initial state ladder) reported in Ustron 2013 Proceedings:
  – *Acta Phys.Polon. B44 (2013) 11, 2179-2187*, [arXiv:1310.6090]
- Also singlet evolution kernels are now almost complete (unpublished).
- It is a major problem to include consistently virtual corrections to exclusive kernels starting from CFP scheme.
- First solution was formulated (unpublished) exploiting recalculated virtual corrections in CFP scheme to non-singlet kernels:
  – *Acta Phys.Polon. B44 (2013) 11, 2197* , [arXiv:1310.7537]
- The above breakthrough is important but points to:
  (i) need of better understanding of the MC distributions in the PS MC,
  (ii)especially their kinematics, definition of the evolution variable etc.
- For the time being this area of the development is not very active:(