Quest for Precision in Simulations for the LHC

Frank Krauss

Institute for Particle Physics Phenomenology
Durham University

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- what the talk is about
- matching & merging with parton showers
- Electroweak corrections
- Revisit Parton Showers
- Revisit Hadronisation
- where we are and where we (should/could/would) go

motivation & introduction

motivation: the need for (more) accurate tools

- to date no survivors in searches for new physics & phenomena

  (a pity, but that's what Nature hands to us)
- push into precision tests of the Standard Model

  (find it or constrain it!)
- statistical uncertainties approach zero

  (because of the fantastic work of accelerator, DAQ, etc.)
- systematic experimental uncertainties decrease

  (because of ingenious experimental work)
- theoretical uncertainties are or become dominant

  (it would be good to change this to fully exploit LHC's potential)

$\Longrightarrow$ more accurate tools for more precise physics needed!

motivation: aim of the exercise

- review the state of the art in precision simulations

(celebrate success)

- highlight missing or ambiguous theoretical ingredients

(acknowledge failure)

- suggest some further studies – experiment and theory

(. . .)

not covered in this talk

(my apologies)

- Status of BSM simulations:
  UFO routinely used in MADGRAPH, HERWIG7, & SHERPA
- Detailed status of individual generators:
  will be discussed tomorrow
- Developments of alternative, specialised code:
  DIPSY (HI), HEJ (FKL MEs), VINCIA (showering), etc.
- Status of analysis framework and long-term data preservation

matching @ (N)NLO

and

merging @ (N)LO

the aftermath of the NLO (QCD) revolution

- establishing a wide variety of automated tools for NLO calculations

  BlackHat, GoSam, MadGraph, NJet, OpenLoops, Recola + automated IR subtraction methods (MadGraph, Sherpa)
- first full NLO (EW) results with automated tools
- technical improvements still mandatory

  (higher multis, higher speed, higher efficiency, easier handling, . . .)
- start discussing scale setting prescriptions

  (simple central scales for complicated multi-scale processes? test smarter prescriptions?)
- steep learning curve still ahead: “NLO phenomenology”

  (example: methods for uncertainty estimates beyond variation around central scale)

prequel: parton showers vs. resummation calculations

- various schemes for various logs in analytic resummation
- concentrate on parton shower instead ⟷ compare with Q_T resummation

(transverse momentum of Higgs boson etc.)

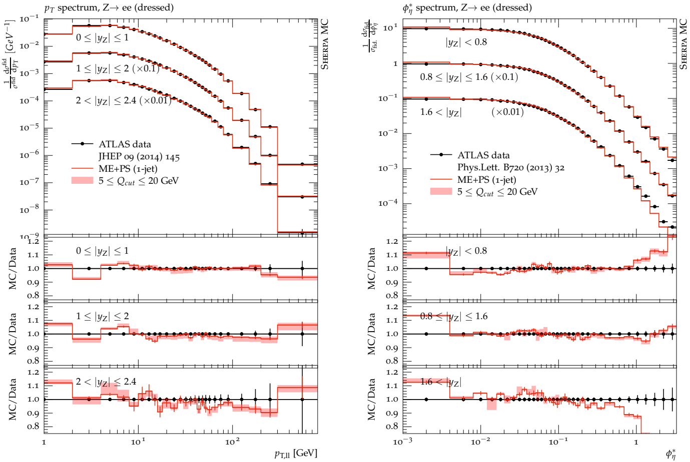
- parametric accuracy by comparing Sudakov form factors:

$$\Delta = \exp\left\{-\int \frac{\mathrm{d}k_\perp^2}{k_\perp^2}\left[A\log\frac{k_\perp^2}{Q^2}+B\right]\right\},$$

  where A and B can be expanded in $\alpha_S(k_\perp^2)$
- showers usually include terms $A_{1,2}$ and B_1 (NLL)
- A_2 often realised by pre-factor multiplying scale $\mu_R \simeq k_\perp$

some parton shower fun with DY

(example of accuracy in description of standard precision observable)



matching at NLO and NNLO

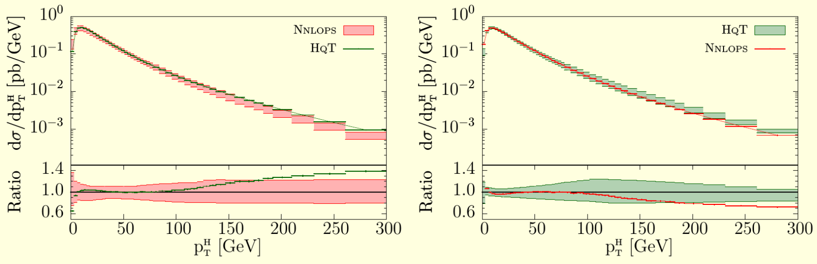
- avoid double-counting of emissions
- two schemes at NLO: MC@NLO and POWHEG
  - mismatches of K factors in transition to hard jet region
  - MC@NLO: $\longrightarrow$ visible structures, especially in $gg \to H$
  - POWHEG: $\longrightarrow$ high tails, cured by h dampening factor
  - well-established and well-known methods

(no need to discuss them any further)

- two schemes at NNLO: MINLO & UN^{2}LOPS (singlets S only)
  - different basic ideas
  - MINLO: $S+j$ at NLO with $p_T^{(S)} \to 0$ and capture divergences by reweighting internal line with analytic Sudakov, NNLO accuracy ensured by reweighting with full NNLO calculation for S production
  - UN^{2}LOPS identifies and subtracts and adds parton shower terms at FO from $S+j$ contributions, maintaining unitarity
  - available for two simple processes only: DY and $gg \to H$

NNLOPs for H production: MINLO

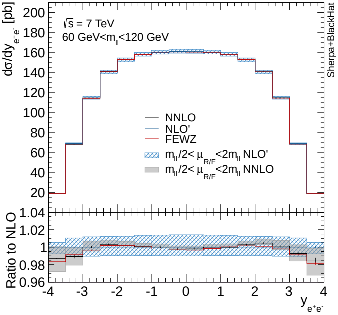
K. Hamilton, P. Nason, E. Re & G. Zanderighi, JHEP 1310

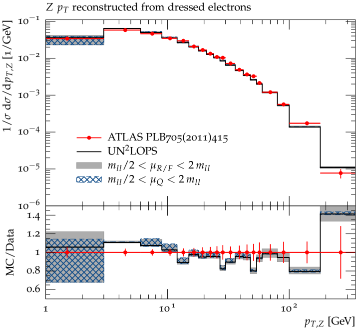


- also available for $Z/W/VH$ production

NNLOPS for Z production: UN^{2}LOPS

S. Hoche, Y. Li, & S. Prestel, Phys.Rev.D90 & D91





- also available for H production

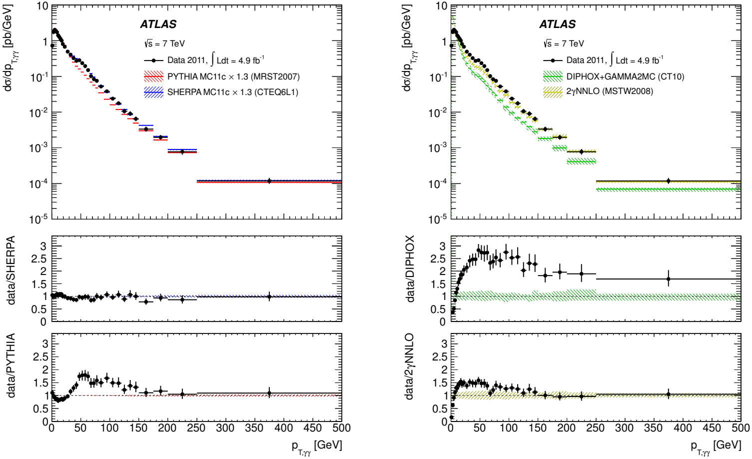
NNLOPS: shortcomings/limitations

- MINLO relies on knowledge of B_2 terms from analytic resummation
  $\longrightarrow$ to date only known for colour singlet production
- MINLO relies on reweighting with full NNLO result
  $\longrightarrow$ one parameter for H (y_H), more complicated for Z, ...

- UN^{2}LOPS relies on integrating single- and double emission to low scales and combination of unresolved with virtual emissions
  $\longrightarrow$ potential efficiency issues, need NNLO subtraction
- UN^{2}LOPS puts unresolved & virtuals in "zero-emission" bin
  $\longrightarrow$ no parton showering for virtuals (?)

merging example: $p_{\perp,\gamma\gamma}$ in MEPS@LO vs. NNLO

(arXiv:1211.1913 [hep-ex])

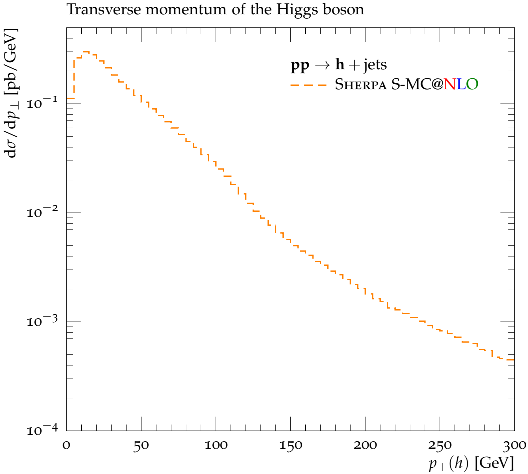


multijet-merging at NLO

- sometimes "more legs" wins over more loops
- basic idea like at LO: towers of MEs with increasing jet multi (but this time at NLO)
- combine them into one sample, remove overlap/double-counting
- maintain NLO and LL accuracy of ME and PS
- this effectively translates into a merging of MC@NLO simulations and can be further supplemented with LO simulations for even higher final state multiplicities
- different implementations, parametric accuracy not always clear

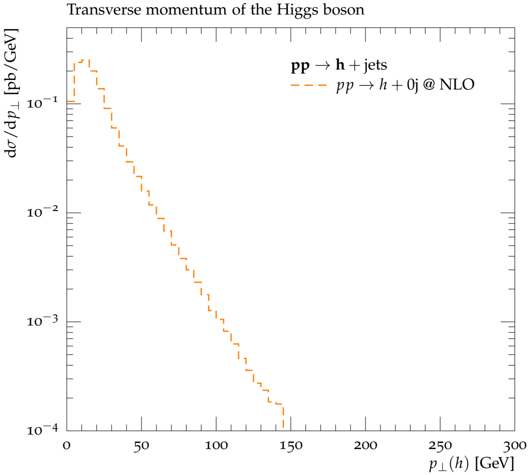
  (MEPS@NLO, FxFx, UNLOPS)
- starts being used, still lacks careful cross-validation

illustration: $p_\perp^H$ in MEPS@NLO



- first emission by MC@NLO

illustration: $p_\perp^H$ in MEPS@NLO



- first emission by MC@NLO , restrict to $Q_{n+1} < Q_\text{cut}$

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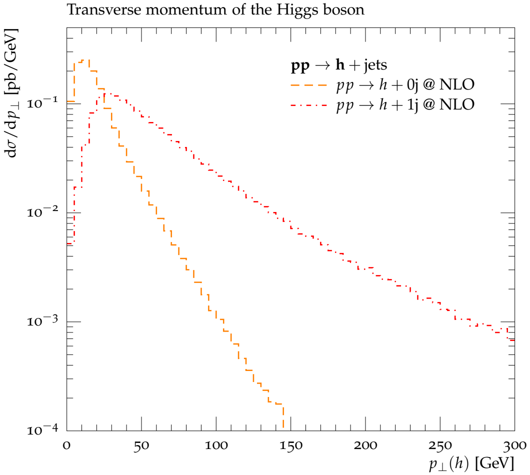

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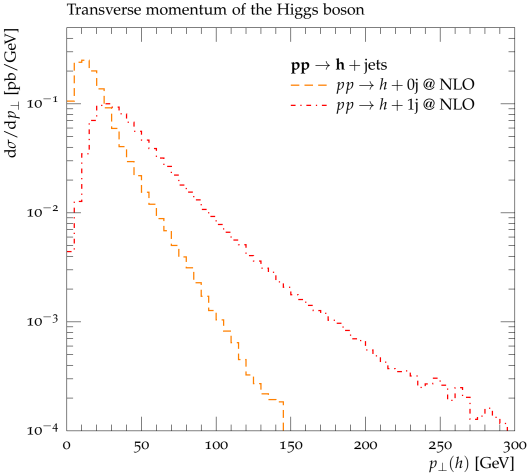

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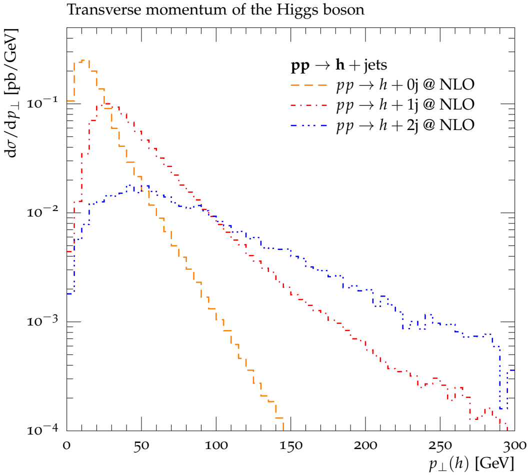

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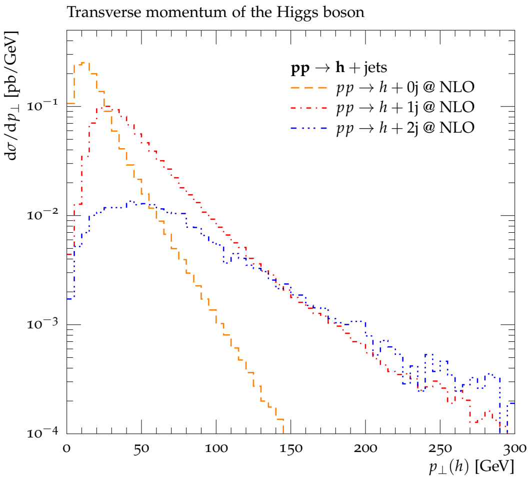

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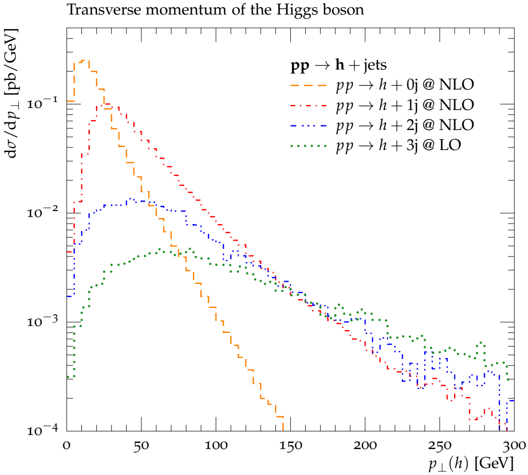

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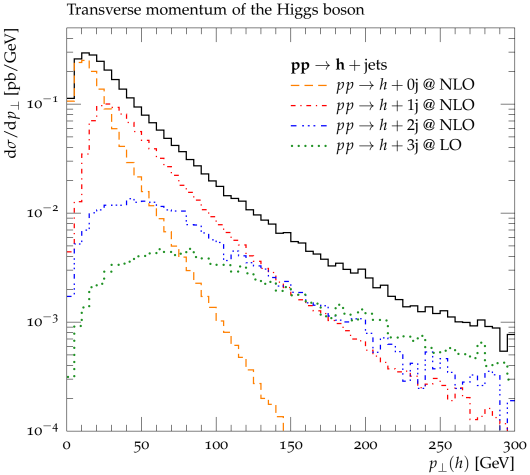

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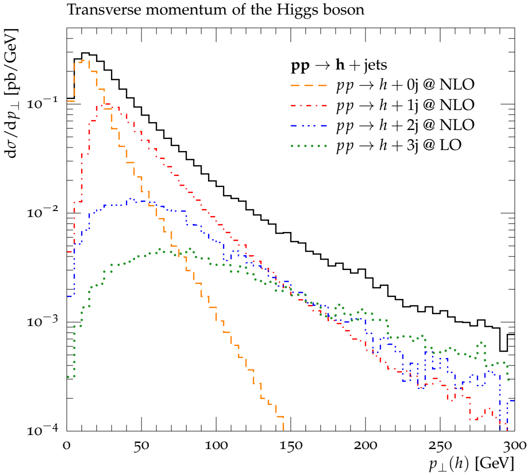
- sum all contributions

illustration: $p_\perp^H$ in MEPS@NLO



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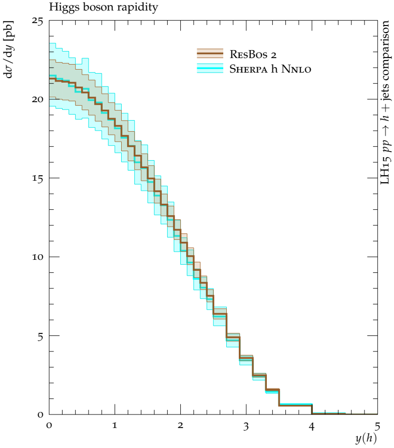
- MC@NLO $pp \to h +$ 2jets for $Q_{n+2} > Q_{\text{cut}}$
- iterate
- sum all contributions
- eg. $p_\perp(h) > 200$ GeV has contributions fr. multiple topologies

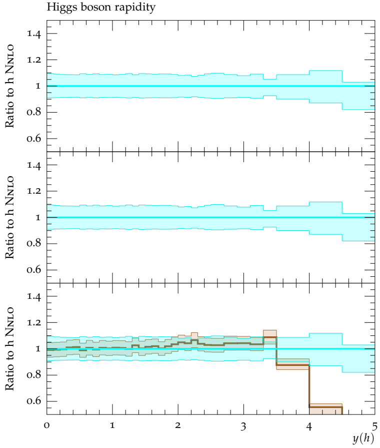
detailed comparison of approaches

in

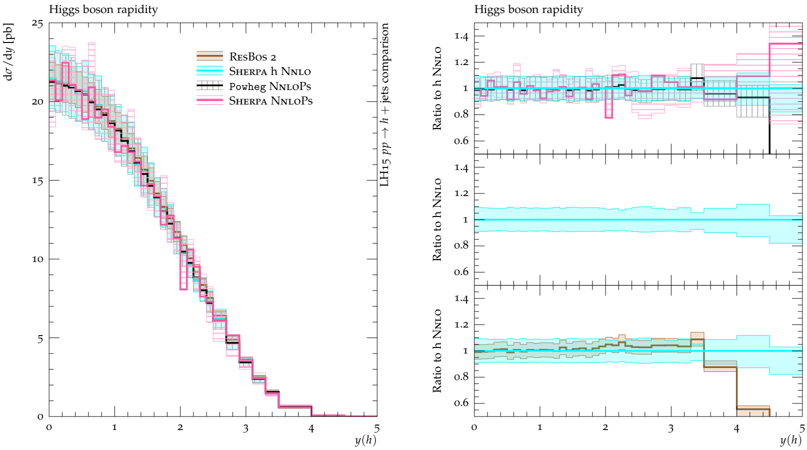
H+jets

inclusive Higgs boson rapidity



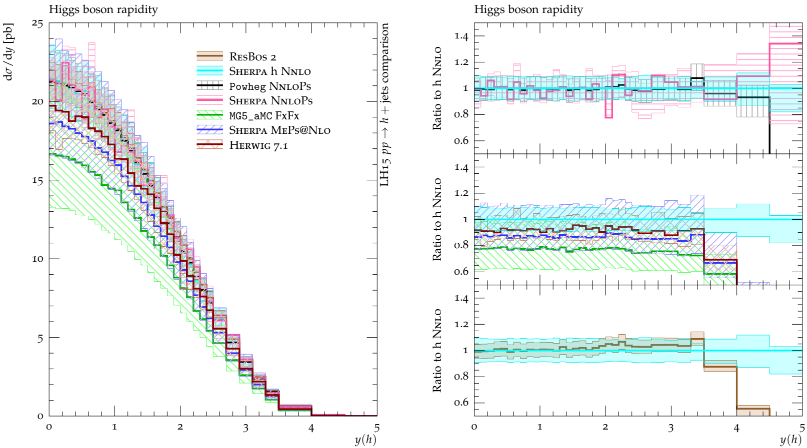


inclusive Higgs boson rapidity



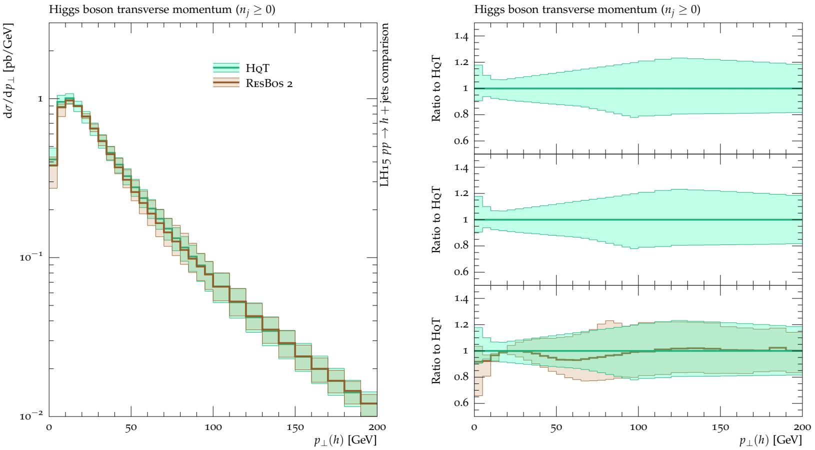
- excellent agreement between NNLO and NNLOPs

inclusive Higgs boson rapidity



- excellent agreement between NNLO and NNLOPs
- multijet merged with NLO normalisation, PDF effects

Higgs boson transverse momentum ($n_j \geq 0$)



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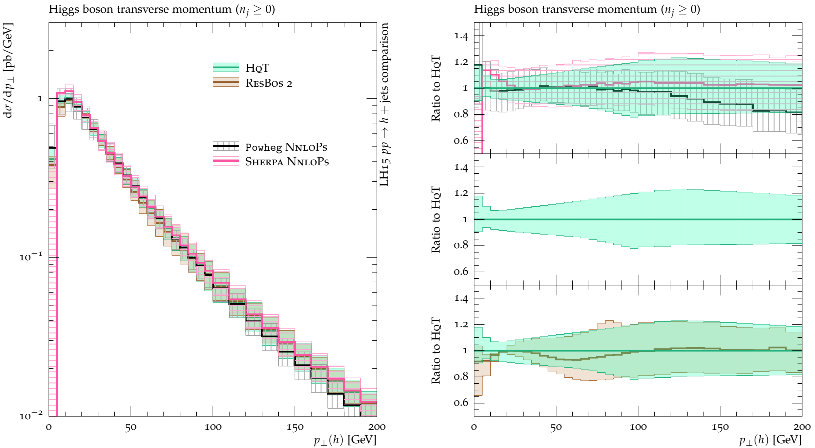
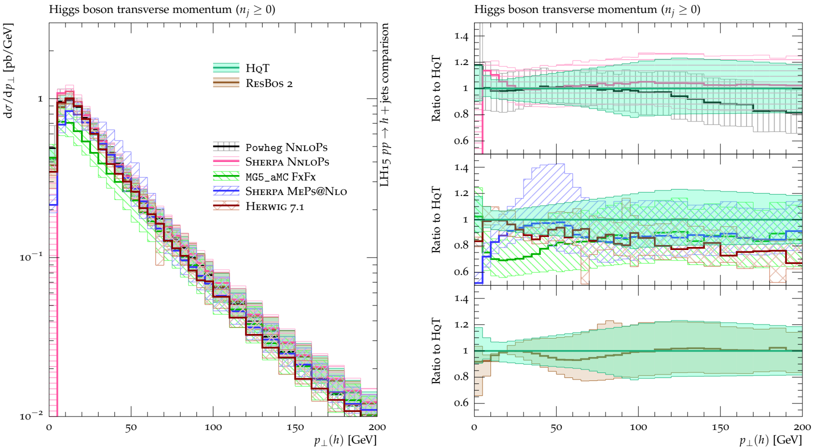


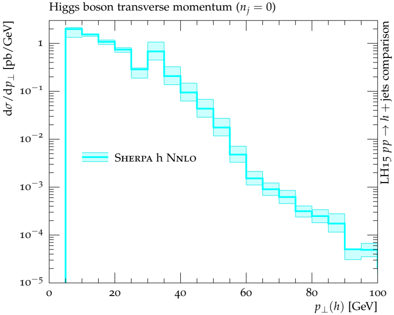
- good agreement between HqT and NNLOPs, scale choice at high $p_\perp$

Higgs boson transverse momentum ($n_j \geq 0$)



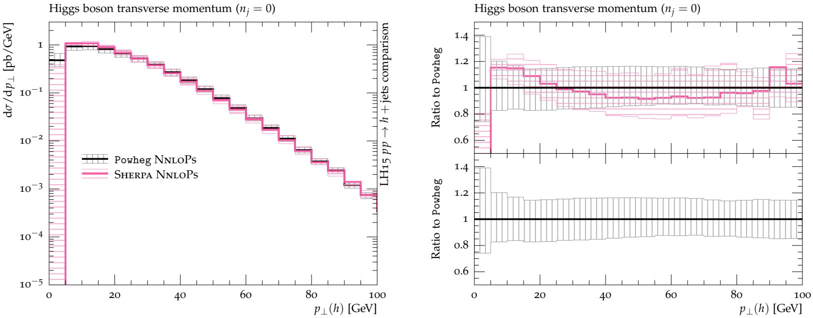
- good agreement between HqT and NNLOPs, scale choice at high $p_\perp$
- multijet merged with NLO normalisation, very different at low $p_\perp$

Higgs boson transverse momentum ($n_j = 0$)



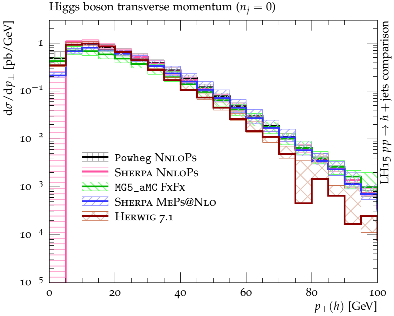
- fixed-order has various unphysical features

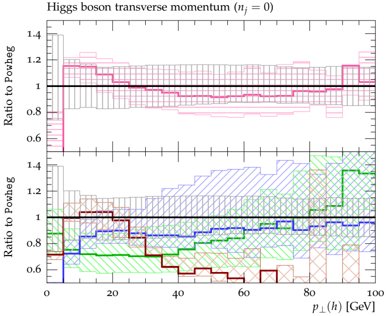
Higgs boson transverse momentum ($n_j = 0$)



- fixed-order has various unphysical features
- good agreement between the NNLOPs

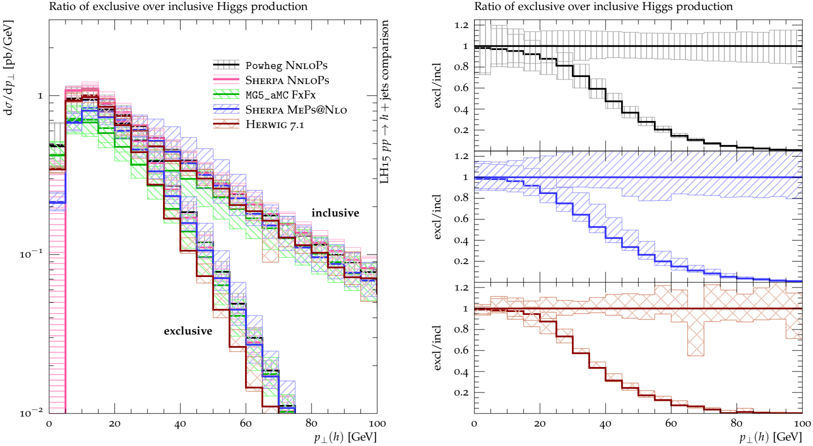
Higgs boson transverse momentum ($n_j = 0$)





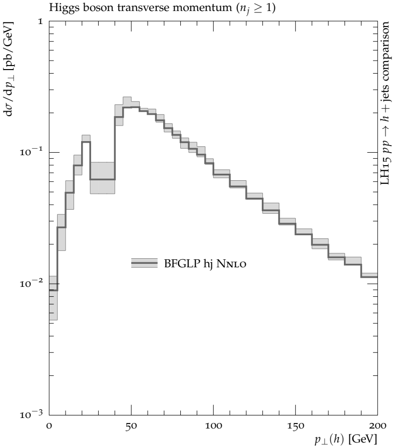
- fixed-order has various unphysical features
- good agreement between the NNLOPs
- multijet merged with NLO normalisation, Herwig7 has much less soft radiation

exclusive over inclusive rate



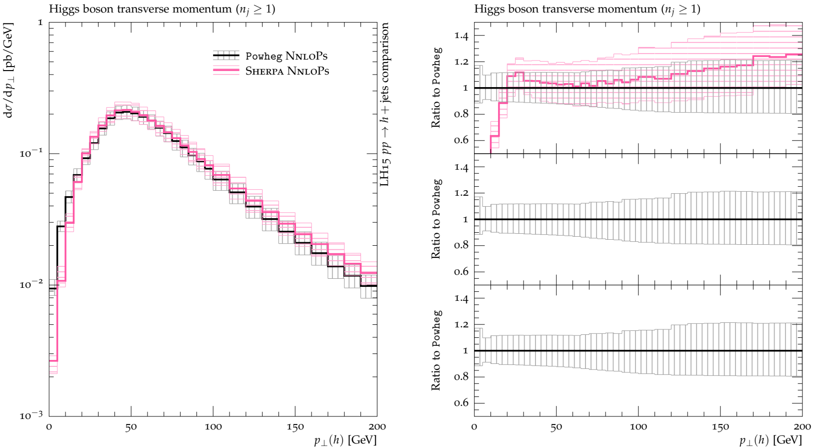
- $\approx 20\%$ of Higgs with $p_\perp = 60\,\text{GeV}$ are not accompanied by a jet

Higgs boson transverse momentum ($n_j \geq 1$)



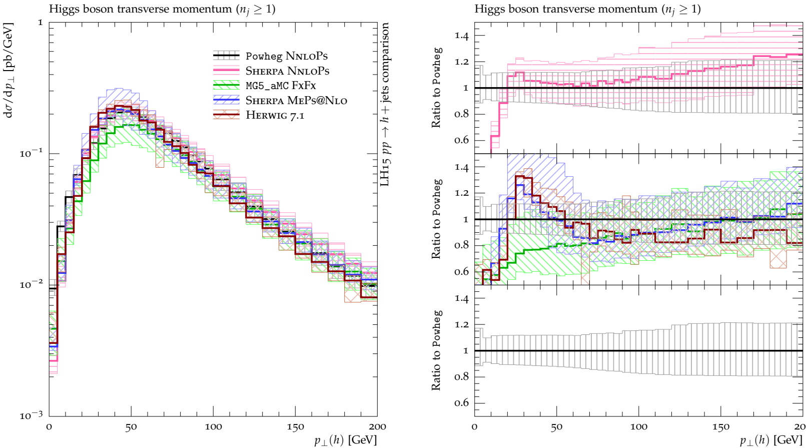
- fixed-order has Sudakov shoulder at $p_\perp^h = 30\,\text{GeV}$ due to jet cut
  here: bins left and right set to average

Higgs boson transverse momentum ($n_j \geq 1$)



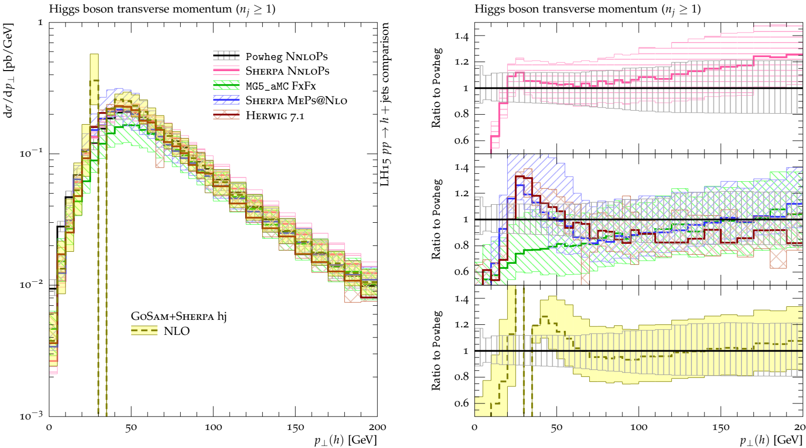
- good agreement between NNLOPS, different scales at large $p_\perp$
- excess of POWHEG as $p_\perp \to 0$ (Higgs strahlung off dijet)

Higgs boson transverse momentum ($n_j \geq 1$)



- multijet merged different shape at $p_\perp \lesssim 60\,\text{GeV}$
- except aMC@NLO_MADGRAPH5 (due to different scales?)

Higgs boson transverse momentum ($n_j \geq 1$)



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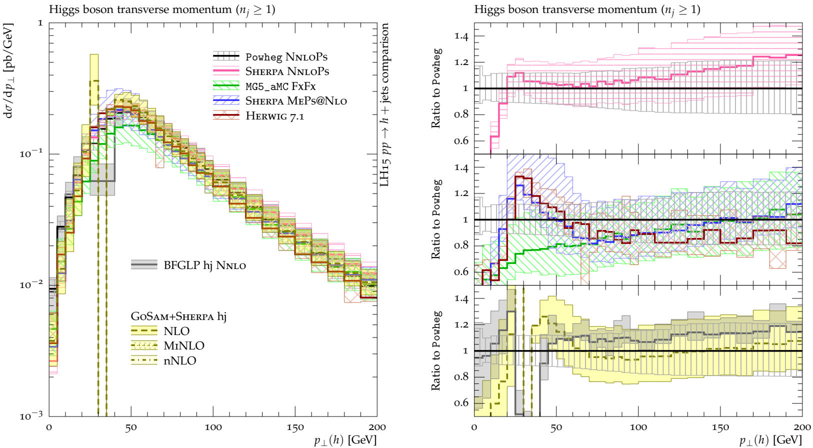
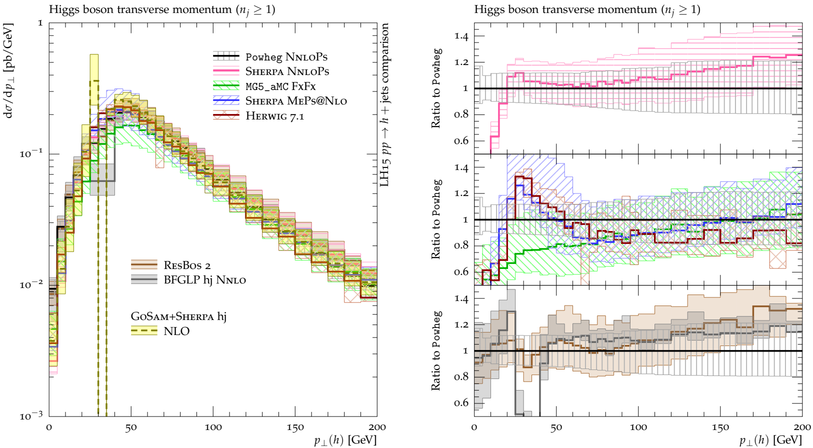
- same as at fixed-order NLO

Higgs boson transverse momentum ($n_j \geq 1$)



- NNLO impacts on shape at $p_\perp \lesssim 60$ GeV
- NLL+NLO resummation gets close to NNLO result

Higgs boson transverse momentum ($n_j \geq 1$)



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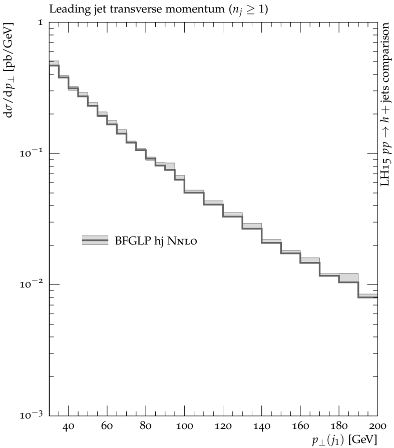
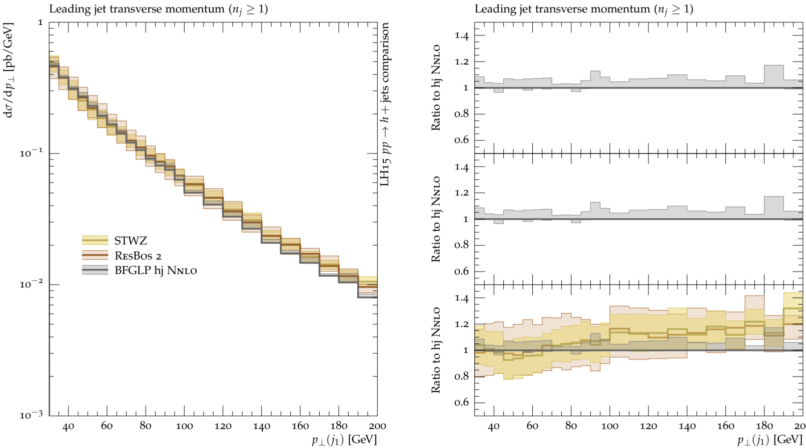
leading jet transverse momentum ($n_j \geq 1$)

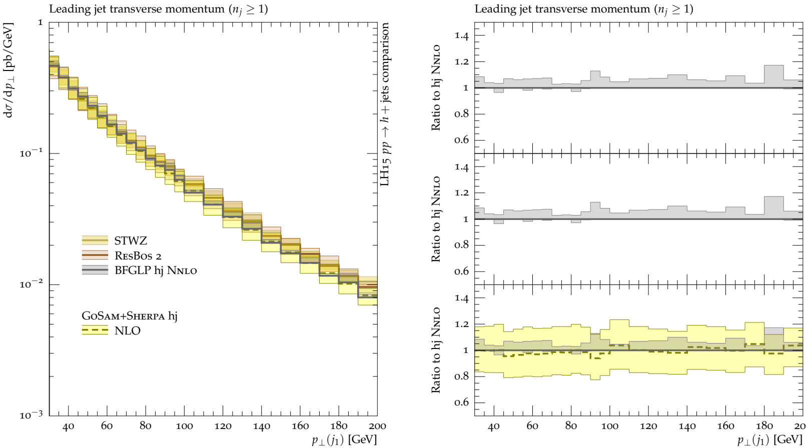


leading jet transverse momentum ($n_j \geq 1$)



- NNLO and NLO show very good convergence for this scale choice

leading jet transverse momentum ($n_j \geq 1$)



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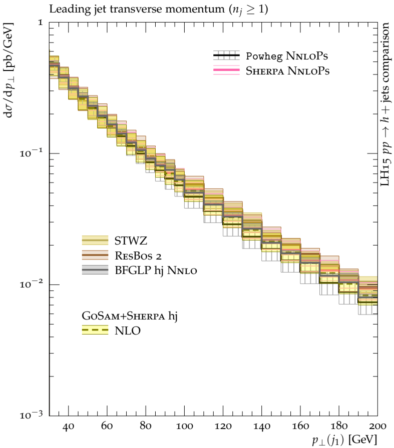
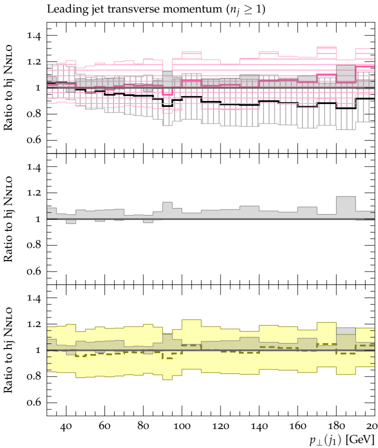
leading jet transverse momentum ($n_j \geq 1$)





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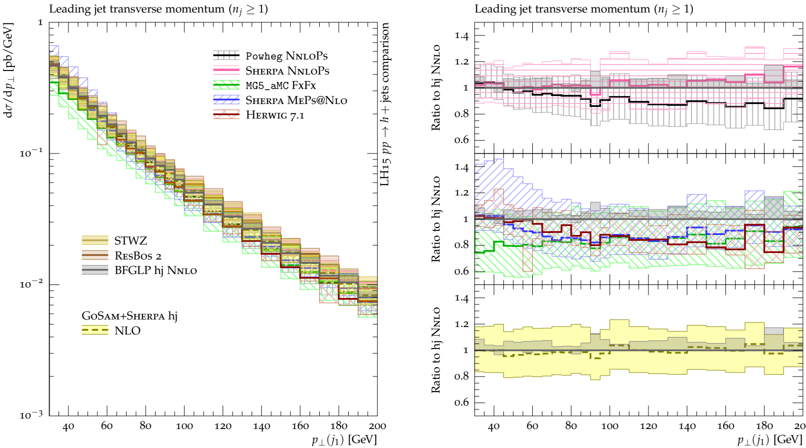
- multijet merged ≈ 20% lower in high-$p_\perp$ (due to showering)

leading jet transverse momentum ($n_j \geq 1$)



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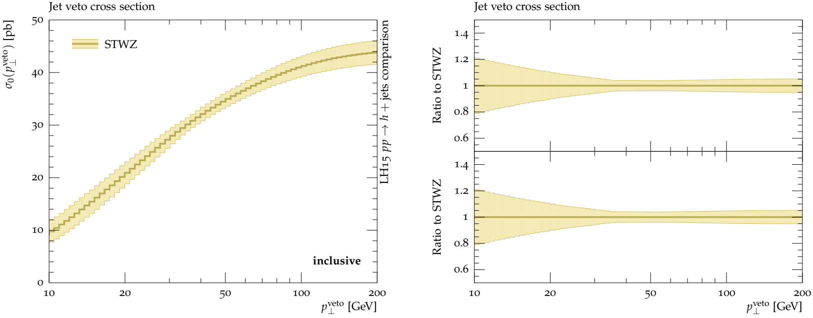
jet vetoed cross sections – inclusive



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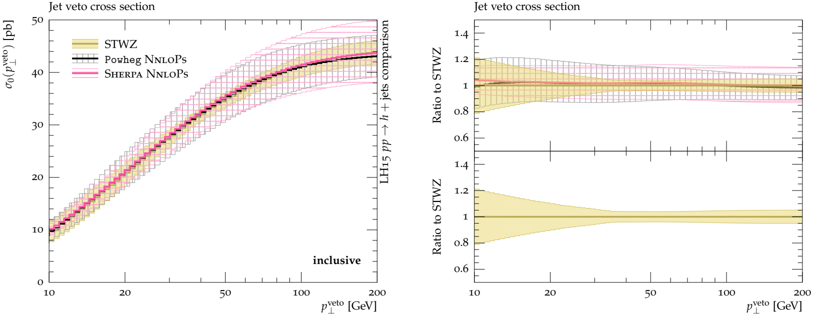
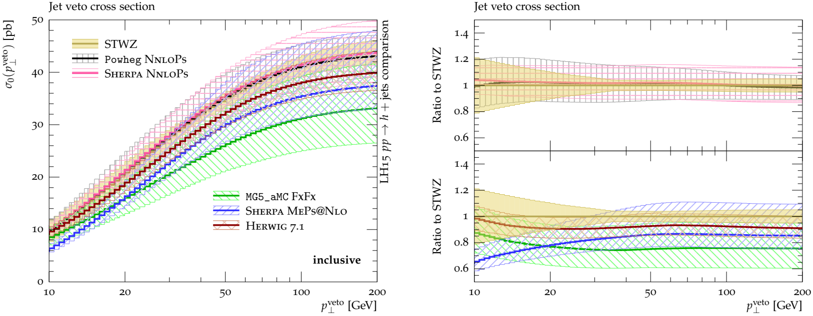


- very good agreement between NNLOPs and STWZ

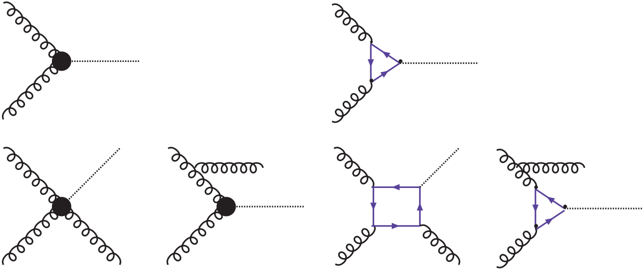
jet vetoed cross sections – inclusive



- very good agreement between NNLOPs and STWZ
- multijet merged with larger spread in shape,
  but within uncertainties once NLO normalisation accounted for
- PS resummation uncertainties nowhere fully assessed

aside: quark mass effects in GGF

- include effects of quark masses

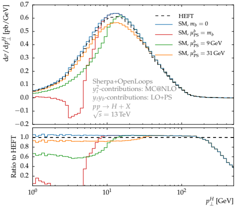


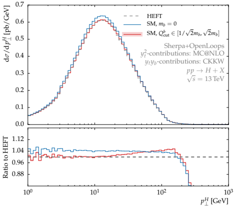
- reweight NLO HEFT with LO ratio:

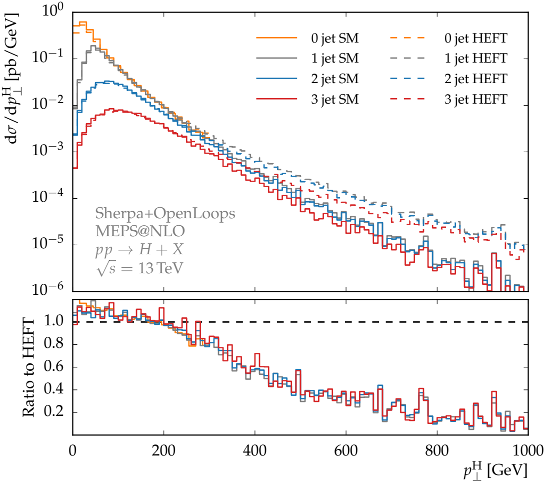
(reweight virtual with Born ratio, real with real ratio)

$$\mathrm{d}\sigma^{(\mathrm{NLO})}_{\mathrm{mass}} \approx \mathrm{d}\sigma^{(\mathrm{NLO})}_{\mathrm{HEFT}} \times \frac{\mathrm{d}\sigma^{(\mathrm{LO})}_{\mathrm{mass}}}{\mathrm{d}\sigma^{(\mathrm{LO})}_{\mathrm{HEFT}}}$$

- example: mass effects in $gg \to H$ (LO merging for b contribution)

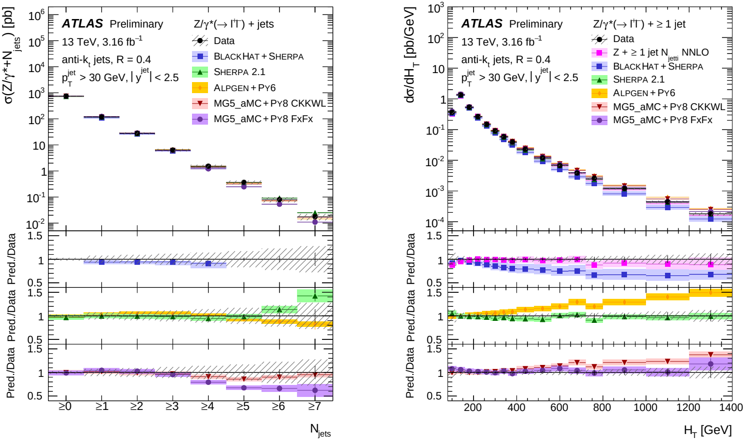






Z+jets at 13 Tev: comparison with ATLAS data

- various merging codes at LO and NLO



including EW corrections

EW corrections

- EW corrections sizeable $\mathcal{O}(10\%)$ at large scales: must include them!
- but: more painful to calculate
- need EW showering & possibly corresponding PDFs

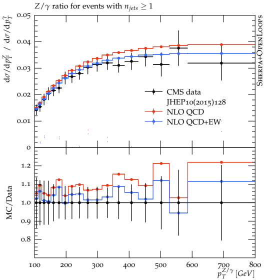
(somewhat in its infancy: chiral couplings)

- example: $Z\gamma$ vs. p_T (right plot)

(handle on $p_\perp^Z$ in $Z\to\nu\bar{\nu}$)

(Kallweit, Lindert, Pozzorini, Schoenherr for LH'15)

- difference due to EW charge of Z
- no real correction (real V emission)
- improved description of $Z\to\ell\ell$



inclusion of electroweak corrections in simulation

- incorporate approximate electroweak corrections in MEPS@NLO
  1. using electroweak Sudakov factors

$$\tilde{\mathrm{B}}_n(\Phi_n) \;\approx\; \tilde{\mathrm{B}}_n(\Phi_n)\,\Delta_{\mathrm{EW}}(\Phi_n)$$

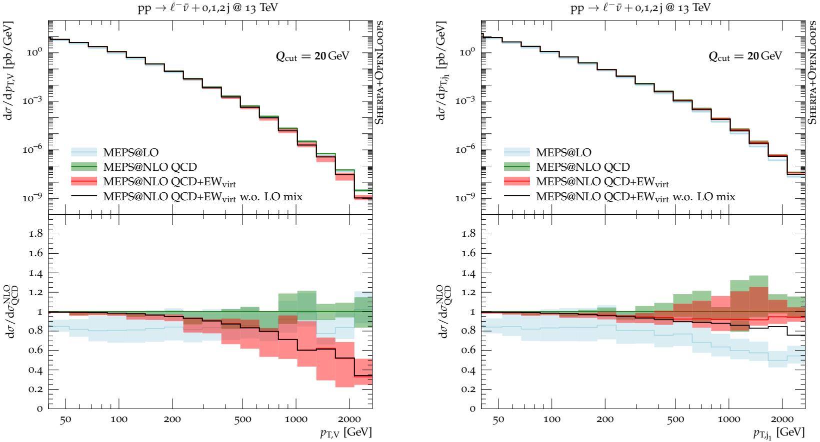
  2. using virtual corrections and approx. integrated real corrections

$$\tilde{\mathrm{B}}_n(\Phi_n) \;\approx\; \tilde{\mathrm{B}}_n(\Phi_n) + \mathrm{V}_{n,\mathrm{EW}}(\Phi_n) + \mathrm{I}_{n,\mathrm{EW}}(\Phi_n) + \mathrm{B}_{n,\mathrm{mix}}(\Phi_n)$$

- real QED radiation can be recovered through standard tools (parton shower, YFS resummation)
- simple stand-in for proper QCD$\oplus$EW matching and merging
  → validated at fixed order, found to be reliable,
  difference $\lesssim 5\%$ for observables not driven by real radiation

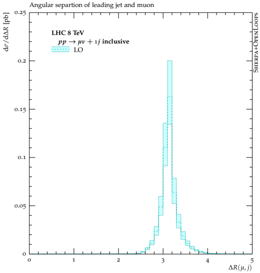
results: $pp \to \ell^- \bar{\nu} + \text{jets}$

(Kallweit, Lindert, Maierhöfer, Pozzorini, Schoenherr JHEP04(2016)021)



⇒ particle level events including dominant EW corrections

NLO EW predictions for $\Delta R(\mu, j_1)$

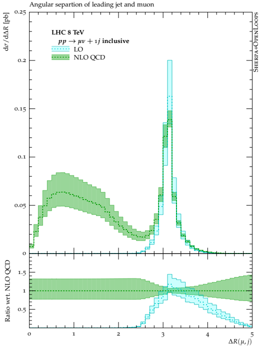


measure collinear W emission?

LHC@8TeV, $p_\perp^{j_1} > 500\,\mathrm{GeV}$, central μ and jet

- LO $pp \to Wj$ with $\Delta\phi(\mu, j) \approx \pi$

NLO EW predictions for $\Delta R(\mu, j_1)$



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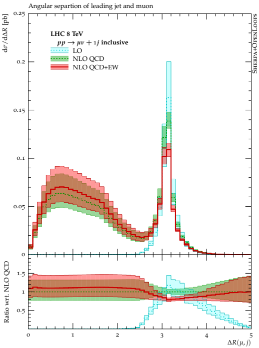

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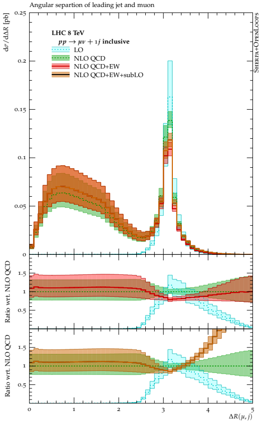

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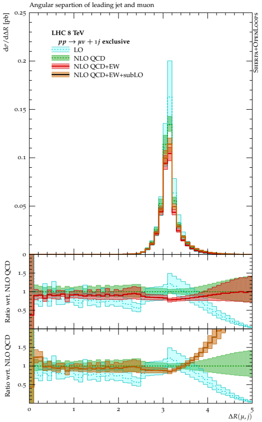

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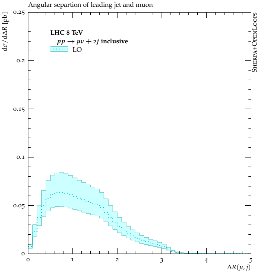

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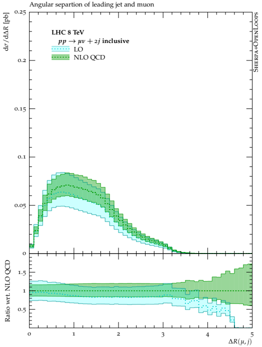

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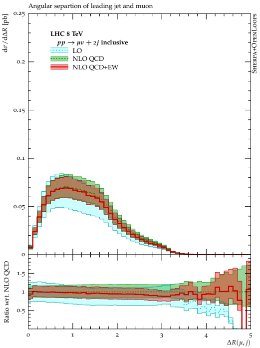

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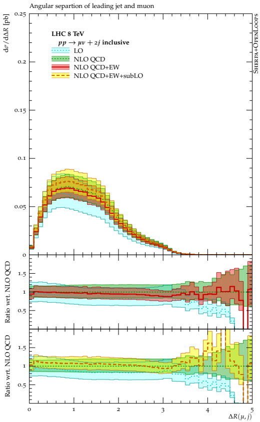

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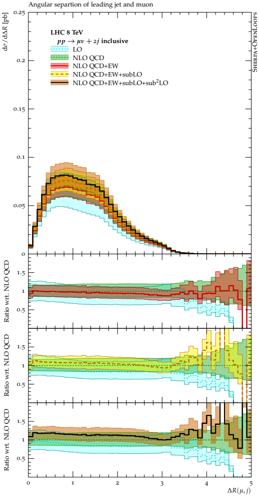

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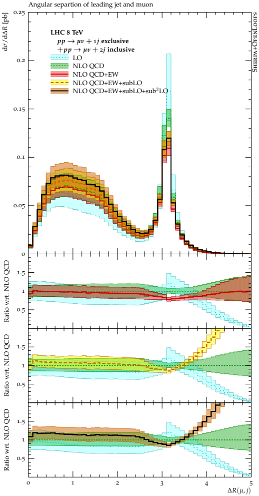
- sub^{2}leading Born (diboson etc) conts. pos.
  $\to$ possible double counting with BG

NLO EW predictions for $\Delta R(\mu, j_1)$



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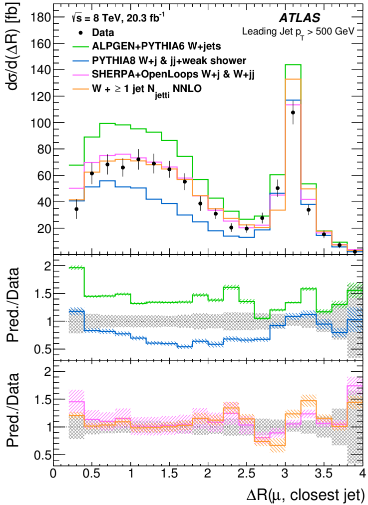
  $\to$ possible double counting with BG
- merge using exclusive sums

NLO EW predictions for $\Delta R(\mu, j_1)$



Data comparison

(M. Wu ICHEP'16, ATLAS arXiv:1609.07045)

- ALPGEN+PYTHIA
  $pp \to W +$ jets MLM merged
  (Mangano et.al., JHEP07(2003)001)
- PYTHIA 8
  $pp \to Wj$ + QCD shower
  $pp \to jj$ + QCD+EW shower
  (Christiansen, Prestel, EPJC76(2016)39)
- SHERPA+OPENLOOPS
  NLO QCD+EW+subLO
  $pp \to Wj/Wjj$ excl. sum
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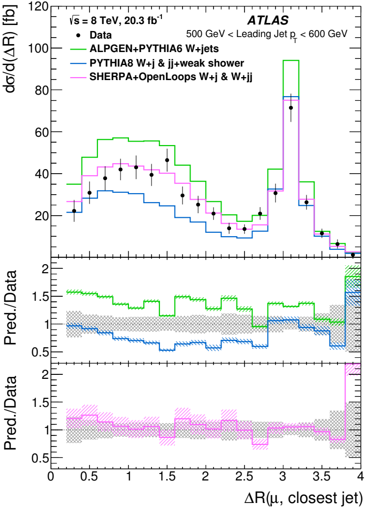

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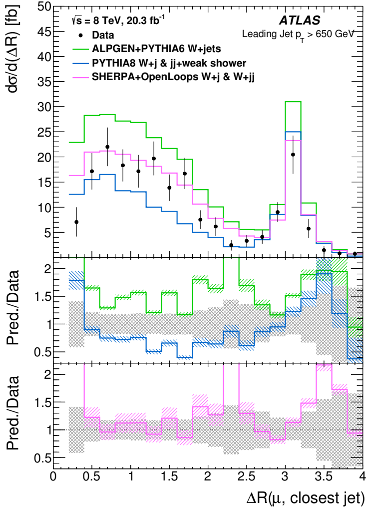

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improving parton showers

another systematic uncertainty

- parton showers are approximations, based on
  leading colour, leading logarithmic accuracy, spin-averaged
- parametric accuracy by comparing Sudakov form factors:

$$\Delta = \exp\left\{-\int \frac{\mathrm{d}k_\perp^2}{k_\perp^2}\left[A\log\frac{k_\perp^2}{Q^2}+B\right]\right\},$$

  where A and B can be expanded in $\alpha_S(k_\perp^2)$
- showers usually include terms $A_{1,2}$ and B_1 (NLL)
- A_2 often realised by pre-factor multiplying scale $\mu_R \simeq k_\perp$

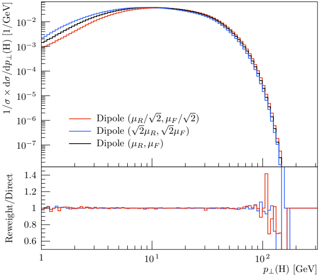
(CMW rescaling: Catani, Marchesini, Webber, Nucl Phys B,349 635)

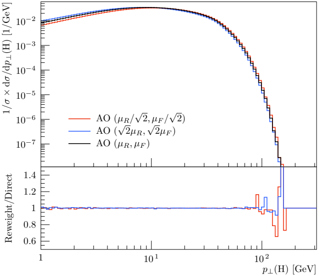
- fixed-order precision necessitates to consistently assess uncertainties from parton showers (quite often just used as black box)
- maybe improve by including higher orders?

event generation (on-the-fly scale variations)

- basic idea: want to vary scales to assess uncertainties
- simple reweighting in matrix elements straightforward
- reweighting in parton shower more cumbersome
  - shower is probabilistic, concept of weight somewhat alien
  - introduce relative weight
  - evaluate (trial-)emission by (trial-)emission

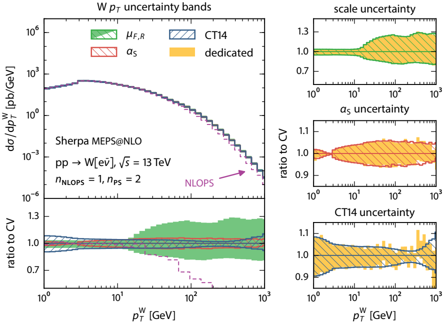
implementation in HERWIG7



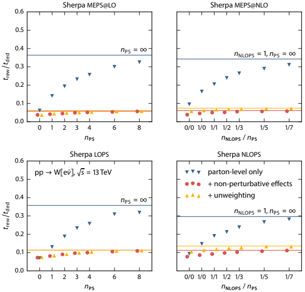


weight variation for W+jets with MEPS@NLO

- uncertainties in $p_\perp^W$



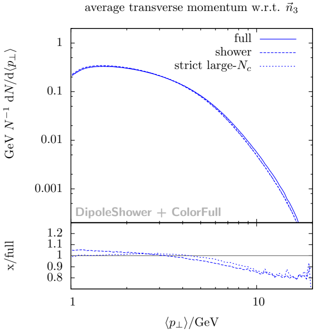
- CPU budget



going beyond leading colour

- start including next-to leading colour

(first attempts by Platzer & Sjodahl; Nagy & Soper)



- also included in 1st emission in SHERPA's MC@NLO

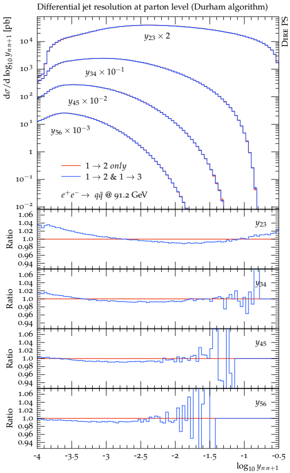
towards higher logarithmic accuracy

- reproduce DGLAP evolution at NLO include all NLO splitting kernels
- corrections to standard 1 → 2 trivial
    - 2-loop cusp term subtracted & combined with LO soft contribution
    - use weighting algorithms

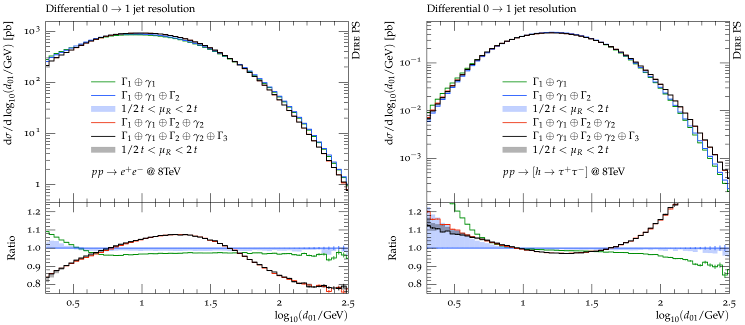
(Hoeche, Schumann, Siegert, 0912.3501)

- new topology at NLO from $q \to \bar{q}$ and $q \to q'$ splittings
- generic 1 → 3 process in parton shower
- first branching treated as soft gluon radiation, second as collinear splitting (to match diagrammatic structure)
- implementation complete and cross-checked (Pythia vs. Sherpa)

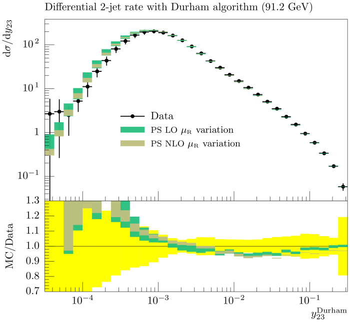
(Catani, Hoeche, FK, Prestel, in prep.)

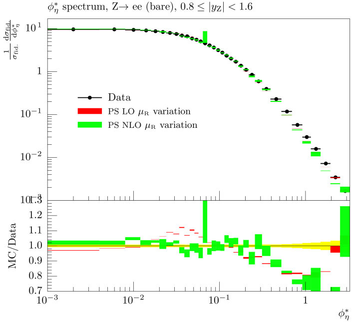


- some first results:
  DY ($pp \to e^+e^-$, left) ggF ($pp \to H \to \tau^+\tau^-$, right)
- added scale uncertainties in parton shower by varying μ_R



- some first results - comparison with data:
  y_{23} at LEP (left) and ϕ^* distribution in Drell-Yan production (right)





hadronisation

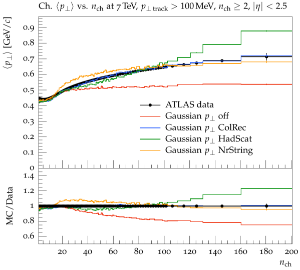
colour reconnections and friends

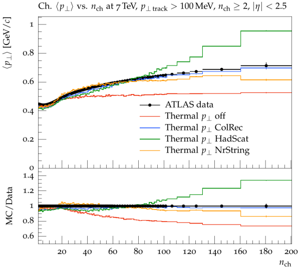
(Fischer, Sjostrand, 1610:09818)

Collective flow observed in pp at LHC. Partly unexpected.
New mechanisms required; could also (partly) replace CR.

Active field, e.g. N. Fischer & TS, arXiv:1610:09818 [hep-ph]:

- Thermal $exp(-p_\perp/T) \to exp(-m_\perp/T)$ hadronic spectrum.
- Close-packed strings $\Rightarrow$ increased string κ or T.
- Dense hadronic gas $\Rightarrow$ hadronic rescattering.



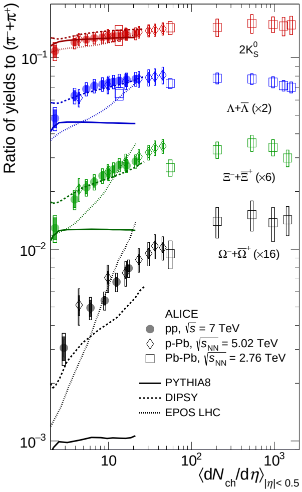


(slide stolen from Torbjorn Sjostrand)

strange strangeness

- universality of hadronisation assumed
- parameters tuned to LEP data
  in particular: strangeness suppression
- for strangeness: flat ratios
  but data do not reproduce this
- looks like $SU(3)$ restoration
  not observed for protons
- needs to be investigated

(ALICE collaboration)



limitations

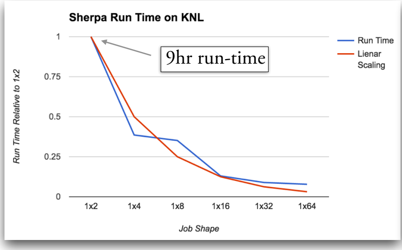
and

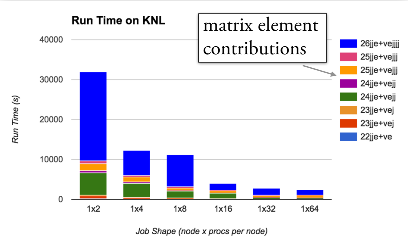
future challenges

limitation: computing short-distance cross sections – LO

(Childers, Uram, LeCompte, Benjamin, Hoeche, CHEP 2016)

- challenge of efficiency on tomorrow's (& today's) computers
- 2000's paradigm: memory free, flops expensive
  (example: 16-core Xeon, 20MB L2 Cache, 64GB RAM)
- 2020's paradigm: flops free, memory expensive & must be managed
  (example: 68-core Xeon KNL, 34MB L2 Cache, 16GB HBM, 96GB RAM)
- may trigger rewrites of code to account for changing paradigm





(figures stolen from Taylor Childers' talk at CHEP)

theory limitations/questions

- we have constructed lots of tools for precision physics at LHC
  $\longrightarrow$ but we did not cross-validate them careful enough (yet)
  $\longrightarrow$ but we did not compare their theoretical foundations (yet)
- we also need unglamorous improvements on existing tools:
  - account for new computer architectures and HPC paradigms
  - systematically check advanced scale-setting schemes (MINLO)
  - automatic (re-)weighting for PDFs & scales
  - scale compensation in PS is simple (implement and check)
- 4 vs. 5 flavour scheme $\longrightarrow$ really?
- how about α_S: range from 0.113 to 0.118

(yes, I know, but still - it bugs me)

$\longrightarrow$ is there any way to settle this once and for all (measurements?)

achievable goals (I believe we know how to do this)

- NLO for loop-induced processes:
    - fixed-order starting, MC@NLO tedious but straightforward
- EW NLO corrections with tricky/time-consuming calculation setup
    - but important at large scales: effect often ∼ QCD, but opposite sign
    - need maybe faster approximation for high-scales (EW Sudakovs)
    - work out full matching/merging instead of approximations
- improve parton shower:
    - beyond (next-to) leading log, leading colour, spin-averaged
    - HO effects in shower and scale uncertainties
    - start including next-to leading colour
    - include spin-correlations → important for EW emissions

more theory uncertainties/issues?

- with NNLOPS approaching 5% accuracy or better:
  - non-perturbative uncertainties start to matter:
    $\longrightarrow$ PDFs, MPIs, hadronization, etc.
  - question (example): with hadronization tuned to quark jets (LEP)
    $\longrightarrow$ how important is the "chemistry" of jets for JES?
    $\longrightarrow$ can we fix this with measurements?
  - example PDFs: to date based on FO vs. data
    $\longrightarrow$will we have to move to resummed/parton showered?

(reminder: LO* was not a big hit, though)

- $g \to q\bar{q}$ at accuracy limit of current parton showers:
  $\longrightarrow$ how bad are $\sim 25\%$ uncertainty on $g \to b\bar{b}$?
  $\longrightarrow$ can we fix this with measurements?

the looming revolution: going beyond NLO

- H in ggF at N^{3}LO (Anastasiou, Duhr and others)
- explosive growth in NNLO (QCD) $2 \to 2$ results

(apologies for any unintended omissions)

  - $t\bar{t}$ (1303.6254; 1508.03585;1511.00549)
  - single-t (1404.7116)
  - VV (1507.06257; 1605.02716;1604.08576; 1605.02716)
  - HH (1606.09519)
  - VH (1407.4747; 1601.00658;1605.08011)
  - $V\gamma$ (1504.01330)
  - $\gamma\gamma$ (1110.2375; 1603.02663)
  - Vj (1507.02850; 1512.01291; 1602.06965; 1605.04295; 1610.07922)
  - Hj (1408.5325; 1504.07922; 1505.03893; 1508.02684; 1607.08817)
  - jj (1310.3993; 1611.01460)
- NLO corrections to $gg \to VV$ (1605.04610)
- WBF at NNLO (1506.02660) and N^{3}LO (1606.00840)
- different IR subtraction schemes:
  N-jettiness slicing, antenna subtraction, sector decomposition,

living with the revolution

- we will include them into full simulations

  (I am willing to place a bet: 5 years at most!)

- practical limitations/questions to be overcome:
  - dealing with IR divergences at NNLO: slicing vs. subtracting

    (I'm not sure we have THE solution yet)

  - how far can we push NNLO? are NLO automated results stable enough for NNLO at higher multiplicity?
  - matching for generic processes at NNLO?

    (MINLO or UN^{2}LOPS or something new?)

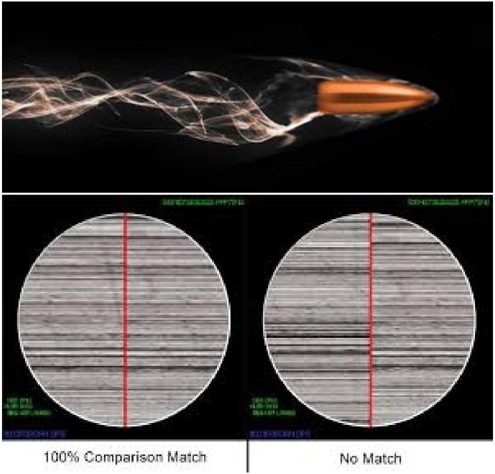
  - more scales (internal or external) complicated – need integrals
- philosophical questions:
  - going to higher power of N often driven by need to include larger FS multiplicity – maybe not the most efficient method
  - limitations of perturbative expansion:

    $\longrightarrow$ breakdown of factorisation at HO (Seymour et al.)

    $\longrightarrow$ higher-twist: compare $(\alpha_S/\pi)^n$ with $\Lambda_{\rm QCD}/M_Z$

outlook

- will need precision for ballistics of smoking guns



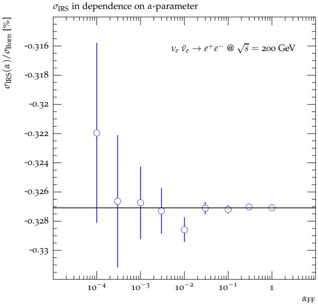
extra: NLO EW subtraction in SHERPA

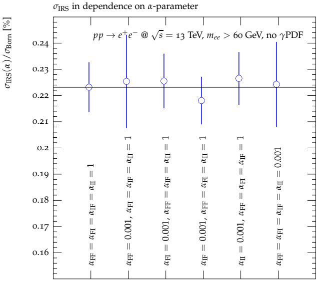
(M. Schoenherr in preparation)

- adapt QCD subtraction (spl. fns. and colour-/spin-correlated MEs)

(Catani, Dittmaier, Seymour, Trocsanyi Nucl.Phys.B627(2002)189-265)

- replacements: $\alpha_s \to \alpha,\ C_F \to Q_f^2,\ C_A \to 0,$
$$T_R \to N_{c,f}\, Q_f^2,\ n_f\, T_R \to \sum_f N_{c,f}\, Q_f^2,$$
$$\frac{\mathbf{T}_{ij}\cdot\mathbf{T}_k}{\mathbf{T}_{ij}^2} \to \frac{Q_{ij}\,Q_k}{Q_{ij}^2}$$


$\sigma_{\rm IRS}$ in dependence on α-parameter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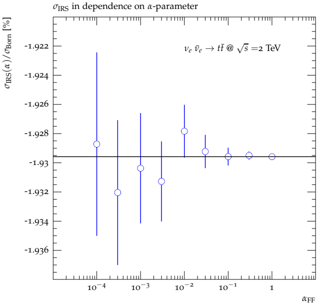

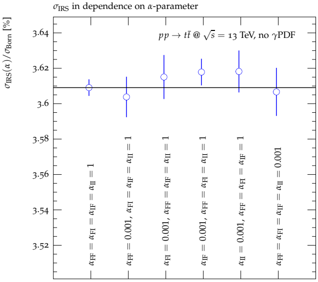

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