Stefano Frixione

A few thoughts on NLO+PS

Higgs Hunting 2014
Paris, 22/7/2014

NLO+PS: why bother?

It is likely a very good idea to use NLO+PS's if at least one of the following conditions is fulfilled:

- Multivariate analyses (BDT, NN, likelihood) are essential, i.e. cut-based ones are not an option
- Lots of backgrounds, (some of which) difficult to tune to data
- Overstretching predictions is highly risky

In general: when experimental results may have a significant theory bias

This boils down to saying that the really crucial thing is:

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$\Longrightarrow$ Using an NLO+PS while neglecting to fully exploit its associated systematics (scale, PDFs, and matching) is a waste of resources

But also:

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NLO+PS results are essentially as easy to obtain as their LO+PS counterparts, owing to the immense and recent progress in *automation techniques*

From the viewpoint of present applications to phenomenology, an NLO+PS is based either on the MC@NLO or on the POWHEG method. I'll now briefly review them

I'll not cover the theoretical activity that aims at improving different aspects of those methods (see e.g. Vincia, GenEva, Nagy&Soper, KRK, Plätzer, ...)

Construction of standalone MC

The generating functional collects all "shower histories" (i.e. kinematic configurations weighted with their probabilities)

$$\mathcal{F}_{\text{MC}} \quad = \quad \mathcal{F}^{(2\to n)} \mathcal{M}^{(b)}(\phi_n) d\phi_n$$

The individual showers emerging from the $2+n$ partons obey:

$$\mathcal{F}(t_I) = \Delta(t_I, t_0) + \int_{t_0}^{t_I} \frac{dt}{t} \Delta(t_I, t) \int dz \frac{\alpha_S}{2\pi} P(z) \mathcal{F}((1-z)^2 t) \mathcal{F}(z^2 t)$$

with parton types understood. When $t = \theta^2 E^2$ one has angular ordering.

The Sudakov form factor is

$$\Delta(t_I, t_0) = \exp\left(- \int_{t_0}^{t_I} \frac{dt}{t} \int dz \frac{\alpha_S}{2\pi} P(z) \right)$$

MCs differ in the choice of shower variables (t and z)

Construction of MC@NLO

$$\mathcal{F}_{\text{MC@NLO}} \quad = \quad \mathcal{F}^{(2\to n+1)}\, d\sigma^{(\mathbb{H})}_{\text{MC@NLO}} + \mathcal{F}^{(2\to n)}\, d\sigma^{(\mathbb{S})}_{\text{MC@NLO}}$$

with the two *finite* short-distance cross sections

$$\begin{aligned} d\sigma^{(\mathbb{H})}_{\text{MC@NLO}} &= d\phi_{n+1}\left(\mathcal{M}^{(r)}(\phi_{n+1}) - \mathcal{M}^{(\text{MC})}(\phi_{n+1})\right) \\ d\sigma^{(\mathbb{S})}_{\text{MC@NLO}} &= \int_{+1} d\phi_{n+1}\left(\mathcal{M}^{(b+v+rem)}(\phi_n) - \mathcal{M}^{(c.t.)}(\phi_{n+1}) + \mathcal{M}^{(\text{MC})}(\phi_{n+1})\right) \end{aligned}$$

that feature the *MC subtraction terms*

$$\boxed{\mathcal{M}^{(\text{MC})} = \mathcal{F}^{(2\to n)}\mathcal{M}^{(b)} + \mathcal{O}(\alpha_S^2\alpha_S^b)}$$

MC subtraction terms are process independent, but MC-dependent
(i.e., those for matching with Herwig and Pythia are different)

Construction of POWHEG

Use the exact phase-space factorization $d\phi_{n+1} = d\phi_n d\phi_r$, and construct

$$\overline{\mathcal{M}}^{(b)}(\phi_n) = \mathcal{M}^{(b+v+rem)}(\phi_n) + \int d\phi_r \left[\mathcal{M}^{(r)}(\phi_{n+1}) - \mathcal{M}^{(c.t.)}(\phi_{n+1})\right]$$

For a *given* p_T, define the (process-dependent) *vetoed* Sudakov

$$\Delta_R(t_I, t_0; p_T) = \exp\left[-\int_{t_0}^{t_I} d\phi'_r \frac{\mathcal{M}^{(r)}}{\mathcal{M}^{(b)}} \Theta(k_T(\phi'_r) - p_T)\right]$$

The short-distance cross section is:

$$d\sigma_{\text{POWHEG}} = d\phi_n \overline{\mathcal{M}}^{(b)}(\phi_n) \left[\Delta_R(t_I, t_0; 0) + \Delta_R(t_I, t_0; k_T(\phi_r)) \frac{\mathcal{M}^{(r)}(\phi_{n+1})}{\mathcal{M}^{(b)}(\phi_n)} d\phi_r\right]$$

- First term ($\mathbb{S}$-type events) strongly suppressed
- $k_T(\phi_r)$ will play the role of hardest emission so far ($\mathbb{H}$-type events)

Attaching (angular-ordered) showers

- One wants the matrix-element-generated p_T to be the hardest
  $\Longrightarrow$ veto emissions harder than p_T during shower

- But this screws up colour coherence

Colour coherence can be restored at the price of a more involved structure

$$\begin{aligned}\mathcal{F}_{\mathsf{POWHEG}}[t_I; p_T] \quad &= \quad \Delta(t_I, t_0) + \int_{t_0}^{t_I} \frac{dt}{t} \int dz \Delta_R(t_I, t; p_T) \frac{\alpha_S}{2\pi} P(z) \\ &\times \mathcal{F}_{\mathsf{V}}((1-z)^2 t; p_T)\, \mathcal{F}_{\mathsf{V}}(z^2 t; p_T)\, \mathcal{F}_{\mathsf{VT}}(t_I, t; p_T)\end{aligned}$$

- $\mathcal{F}_{\mathsf{V}}(t; p_T)$ are *vetoed* showers. Evolve down to t_0, with all emissions constrained to have a transverse momentum smaller than p_T

- $\mathcal{F}_{\mathsf{VT}}(t_I, t; p_T)$ are *vetoed-truncated* showers. Evolve from t_I down to t (i.e., *not* t_0) along the hardest line. On top of that, they are vetoed

To reduce the impact of the exponentiation of the full real matrix element, one introduces the following variant

$$d\sigma_{\mathrm{POWHEG}}^{(\mathrm{damp})} = d\phi_n \overline{\mathcal{M}}_S^{(b)} \left\{ \Delta_R^S \frac{\mathcal{M}_S^{(r)}}{\mathcal{M}^{(b)}} + \mathcal{M}_F^{(r)} \right\} d\phi_r$$

with:

$$\mathcal{M}^{(r)} = \mathcal{M}_S^{(r)} + \mathcal{M}_F^{(r)} = F(p_T)\mathcal{M}^{(r)} + (1 - F(p_T))\mathcal{M}^{(r)}$$

$$(1 - F(p_T))\mathcal{M}^{(r)} \longrightarrow \text{finite} \qquad p_T \longrightarrow 0$$

To maintain the NLO accuracy, one must define:

$$\overline{\mathcal{M}}_S^{(b)} = \overline{\mathcal{M}}^{(b)} \left(\mathcal{M}^{(r)} \longrightarrow \mathcal{M}_S^{(r)} \right) \qquad \Delta_R^S = \Delta_R \left(\mathcal{M}^{(r)} \longrightarrow \mathcal{M}_S^{(r)} \right)$$

Features

$\mathrm{MC@NLO} = \mathrm{POWHEG} + \mathcal{O}(\alpha_S^2 \alpha_S^b) + \mathrm{logs}$ (with or without damp)

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  - Exponentiation of real matrix elements
  - Use of $\overline{\mathcal{M}}^{(b)}$, which "moves" the $p_T = 0$ K factor to $p_T > 0$ *before* showering

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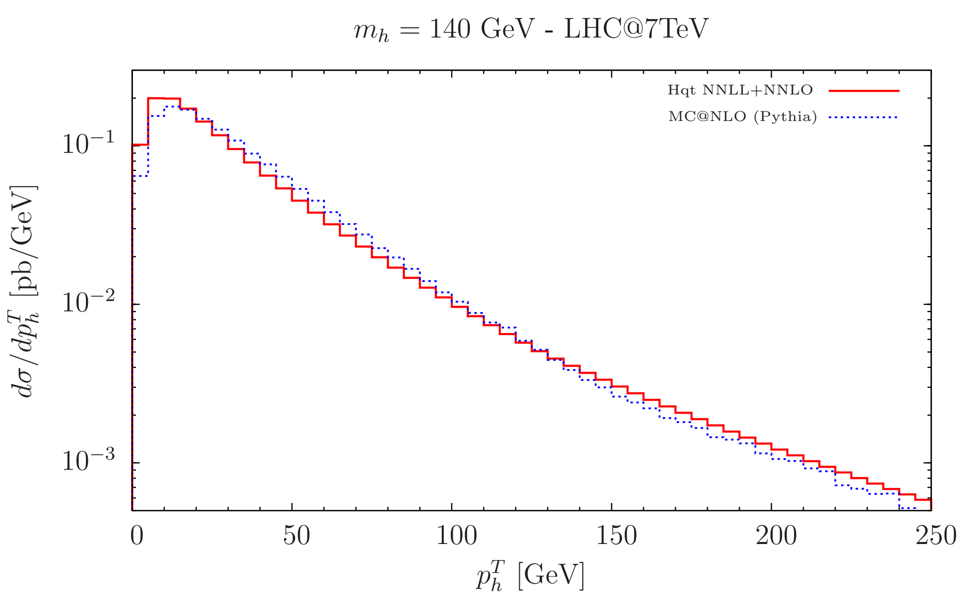
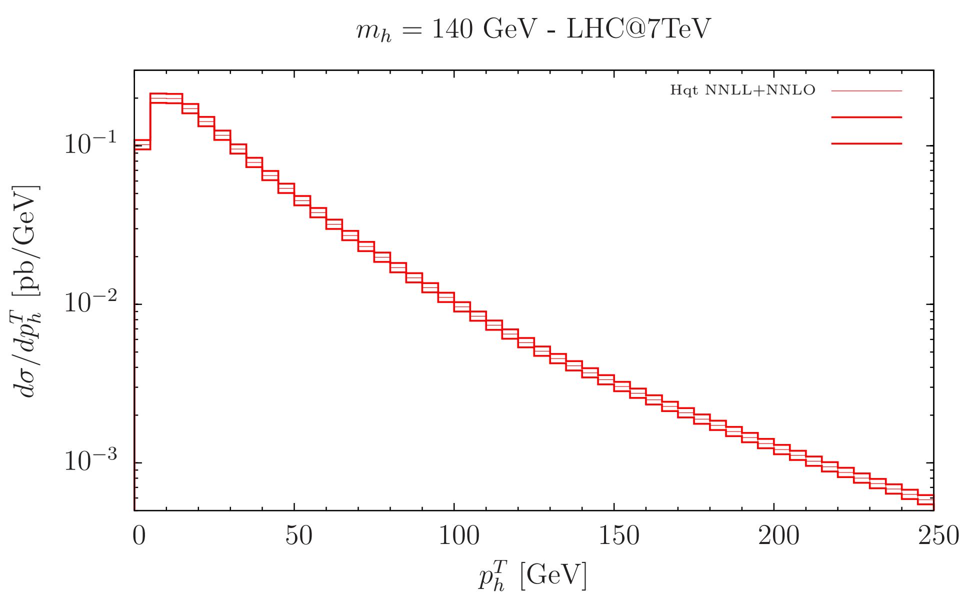
These differences are generally small (for inclusive variables at least).
$gg \to H$ is a spectacular counterexample

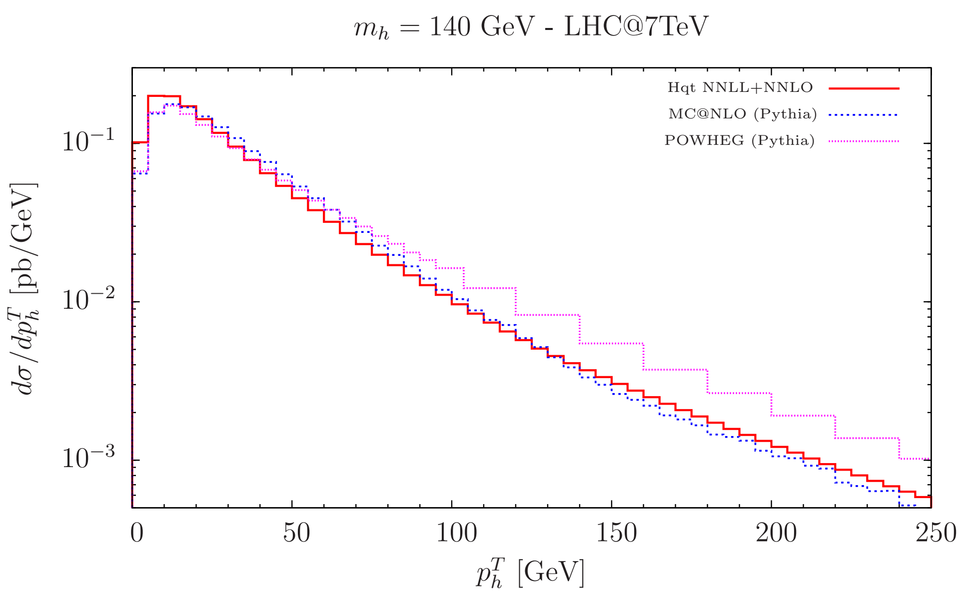
$p_T(H)$ in $gg \to H$

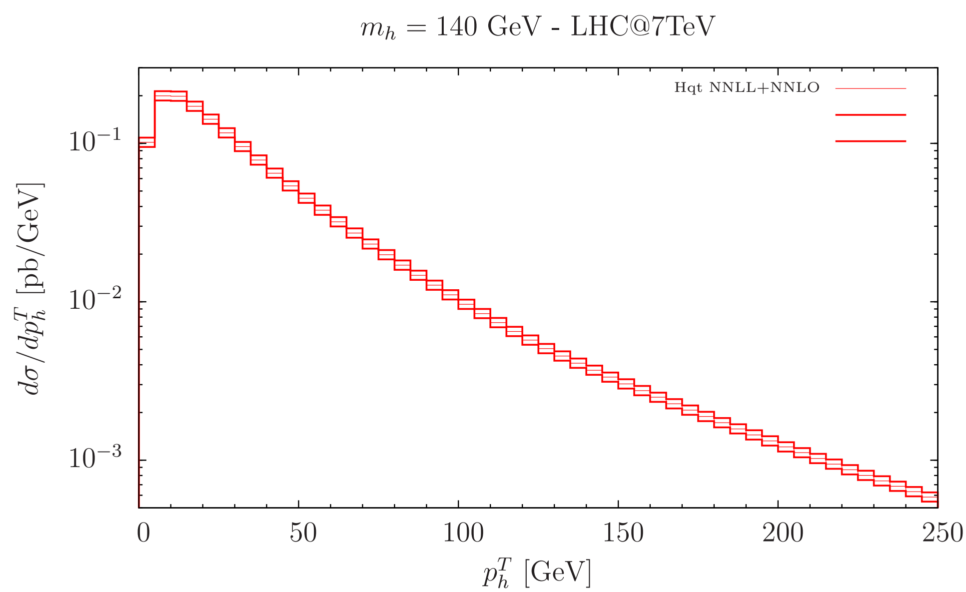




Note: matrix elements in MC@NLO (and POWHEG) are up to $\mathcal{O}(\alpha_S^3)$, in HqT up to $\mathcal{O}(\alpha_S^4)$. MC@NLO and HqT compatible within theory uncertainty

$p_T(H)$ in $gg \to H$





The POWHEG tail is more than a factor of two higher than the MC@NLO one

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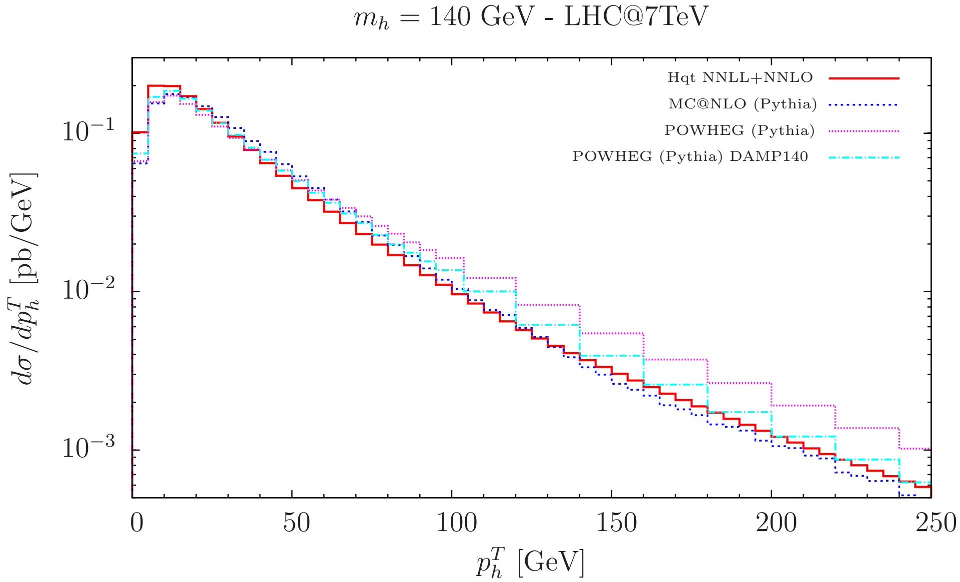
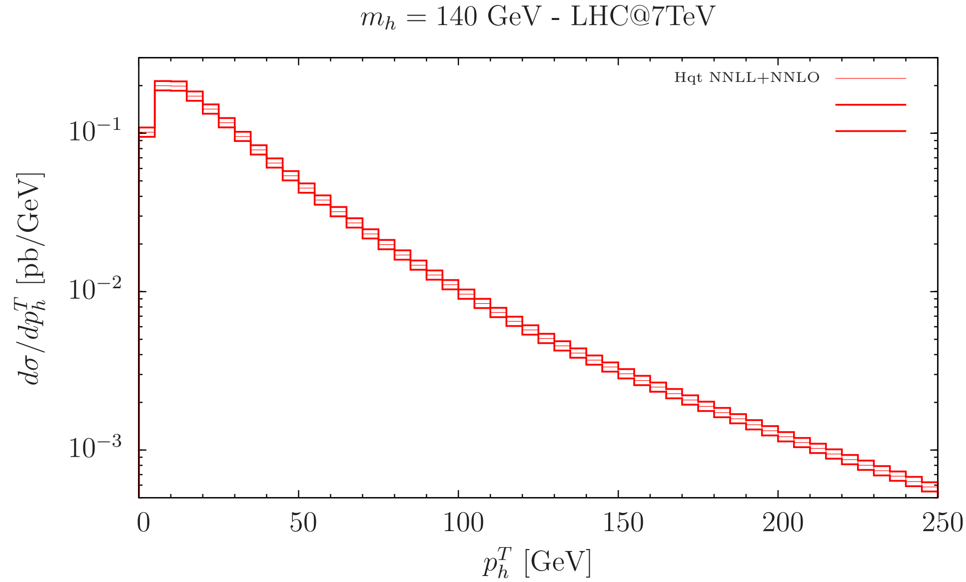




Use of $F(p_T) \neq 1$ brings the POWHEG curve significantly down.
Note that this is formally an $\mathcal{O}(\alpha_S^4)$ effect

Take-home messages:

- Small-p_T region: MC@NLO relies entirely on the MC, POWHEG uses own Sudakov for the first emission

- When matched to angular-ordered MCs, POWHEG must use vetoed-truncated showers to have the same *leading* logarithmic structure of the underlying MC

- In POWHEG, $F(p_T)$ ($\leftrightarrow$ `hfact`) must be treated:
  - either as a tuning parameter, and its role discussed as such
  - or as a source of systematics, to be included in the theory uncertainty

As an aside, a further couple of points:

- MC@NLO and POWHEG do *not* have the same kind of scale and PDF uncertainties
- The so-called S-MC@NLO matching is *identical* to MC@NLO. It employs a *parton shower* which is not the same as that used for LO simulations in Sherpa (see e.g. page 49 of 1405.0301)

AUTOMATION

Automation

There were very few people working on this in 2008

Automation is now a proper field, with many large groups obtaining results at a very remarkable rate

MadFKS (Frederix, Frixione, Maltoni, Stelzer 0908.4272), HELAC (Czakon, Papadopoulos, Worek 0905.0883), MadDipole (Frederix, Gehrmann, Greiner 1004.2905, 0808.2128), SHERPA (Gleisberg, Krauss 0709.2881), MadLoop (Hirschi, Frederix, Frixione, Garzelli, Maltoni, Pittau, 1103.0621), BlackHat (Berger, Bern, Dixon, Febres Cordero, Forde, Gleisberg, Ita, Kosower, Maitre 1009.2338), Rocket (Ellis, Giele, Kunszt, Melnikov, Zanderighi 0810.2762), HELAC-NLO (Bevilacqua, Czakon, Garzelli, van Hameren, Kardos, Papadopoulos, Pittau, Worek, 1110.1499), GoSam (Cullen, Greiner, Heinrich, Luisoni, Mastrolia, Ossola, Reiter, Tramontano, 1111.2034), OpenLoops (Cascioli, Maierhofer, Pozzorini, 1111.5206)

+ too_many_papers_to_cite... (search for the authors above)

What I am involved in:

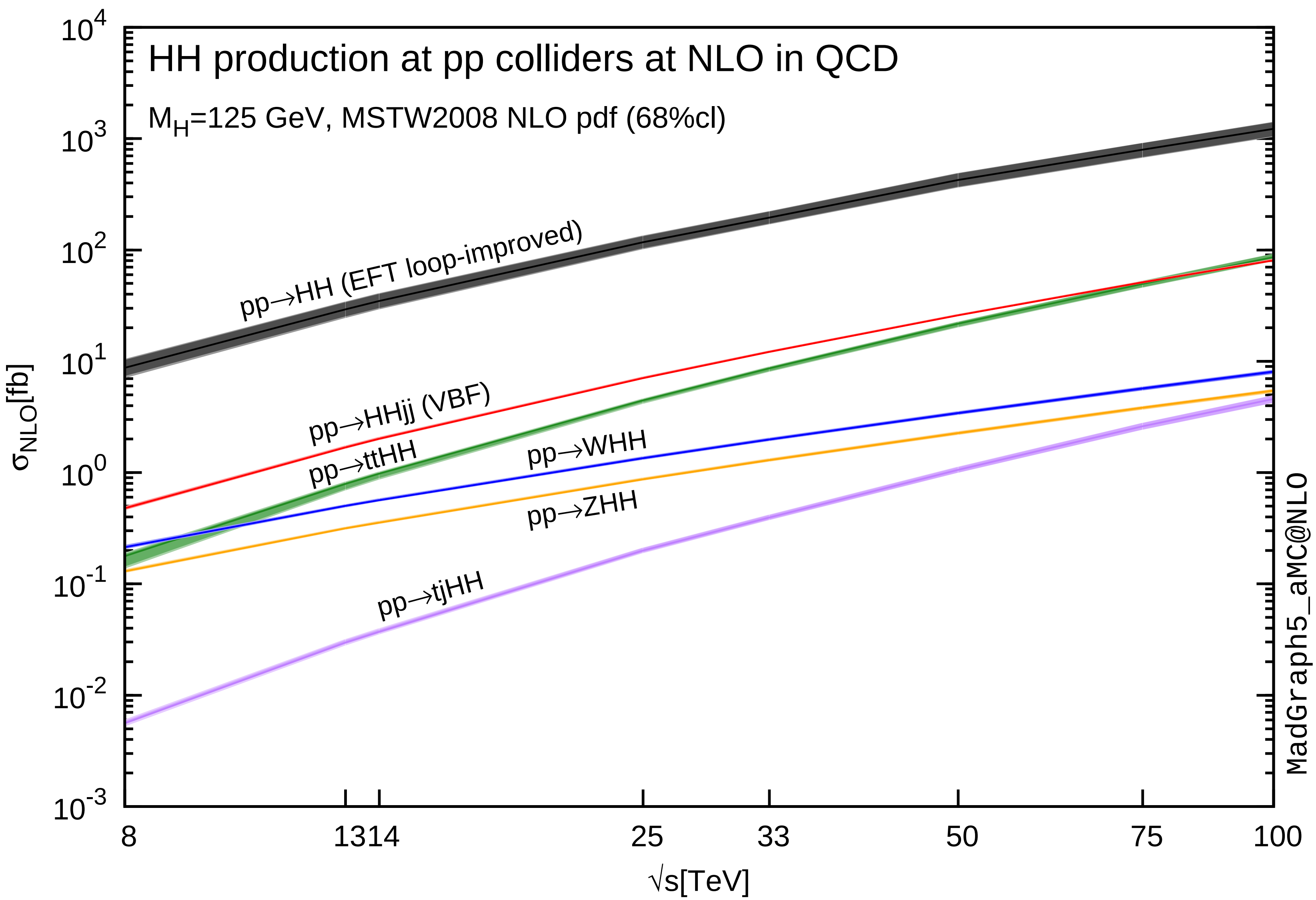
MadGraph5_aMC@NLO [arXiv:1405.0301]

(Alwall, Frederix, Frixione, Hirschi, Maltoni, Mattelaer, Shao, Stelzer, Torrielli, Zaro)

- Computations at the LO and the NLO
- Without or with (MC@NLO) matching to parton showers
- With or without multi-parton merging

Provides *all* ingredients to the above computations in a single package (the *only* example of its kind)

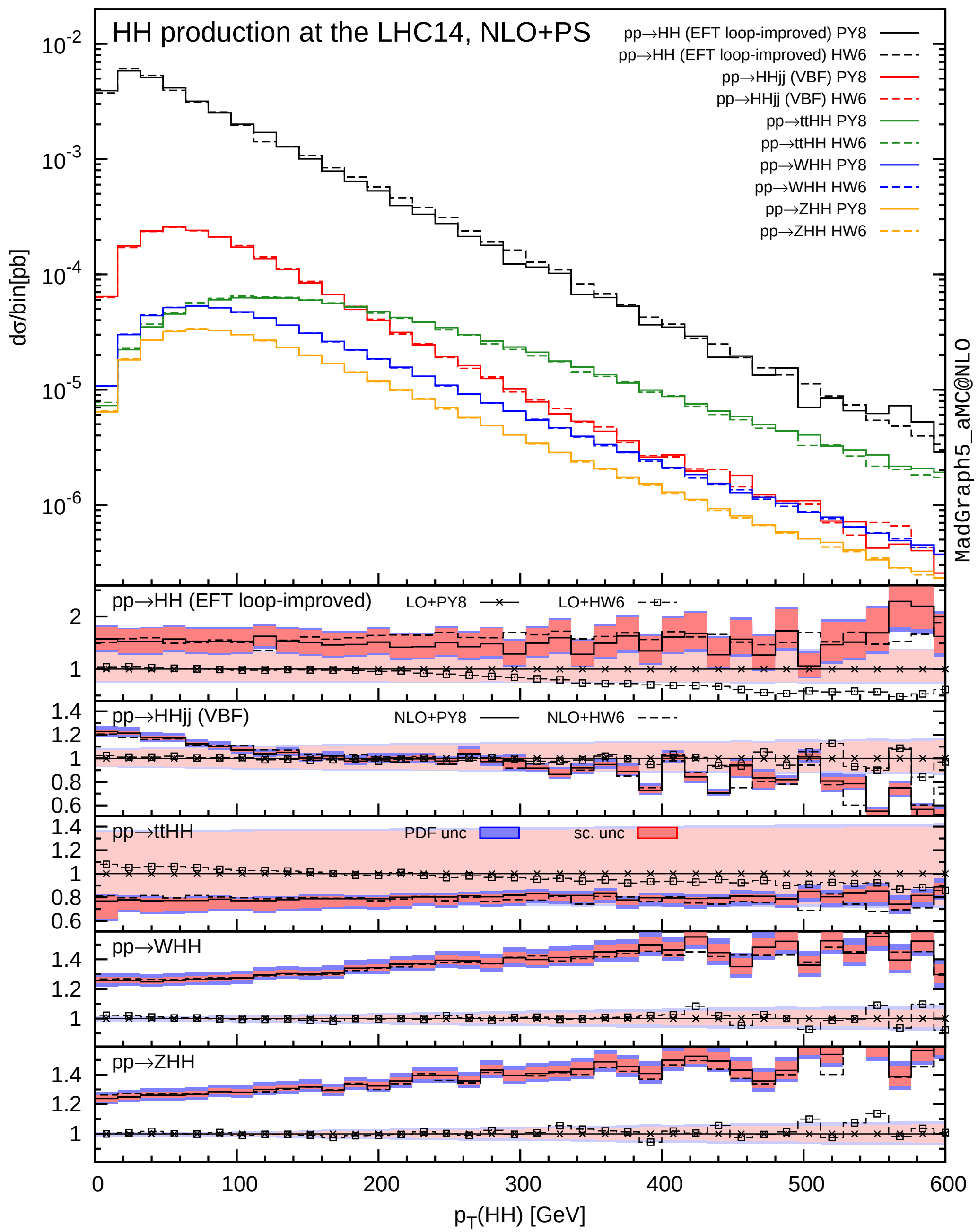
Recent examples $\longrightarrow$



SM at NLO: thickness of lines is scale+PDF uncertainties

arXiv:1401.7340 [hep-ph] ⟶ See M. Zaro's talk

(Frederix, Frixione, Hirschi, Maltoni, Mattelaer, Torrielli, Vryonidou, Zaro)

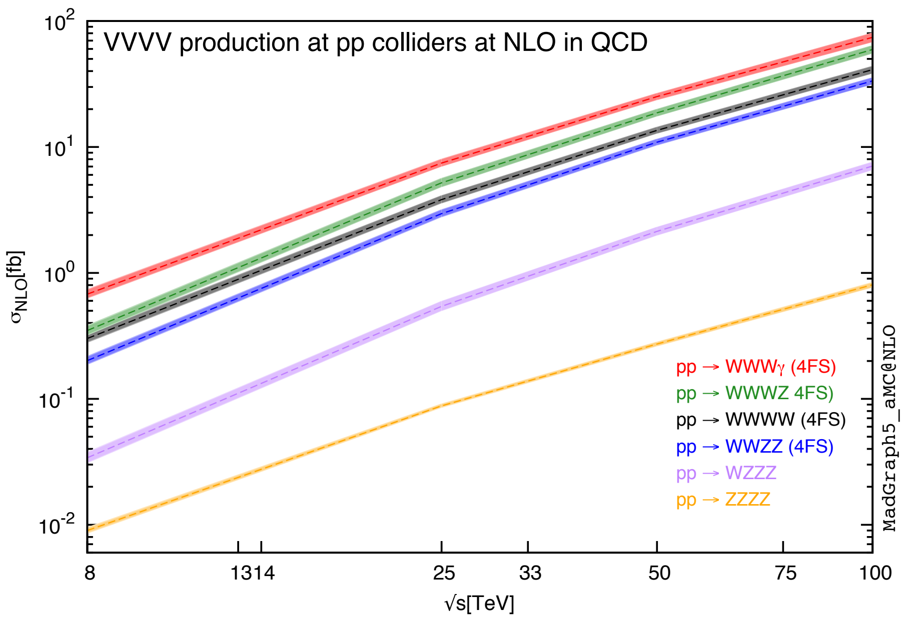


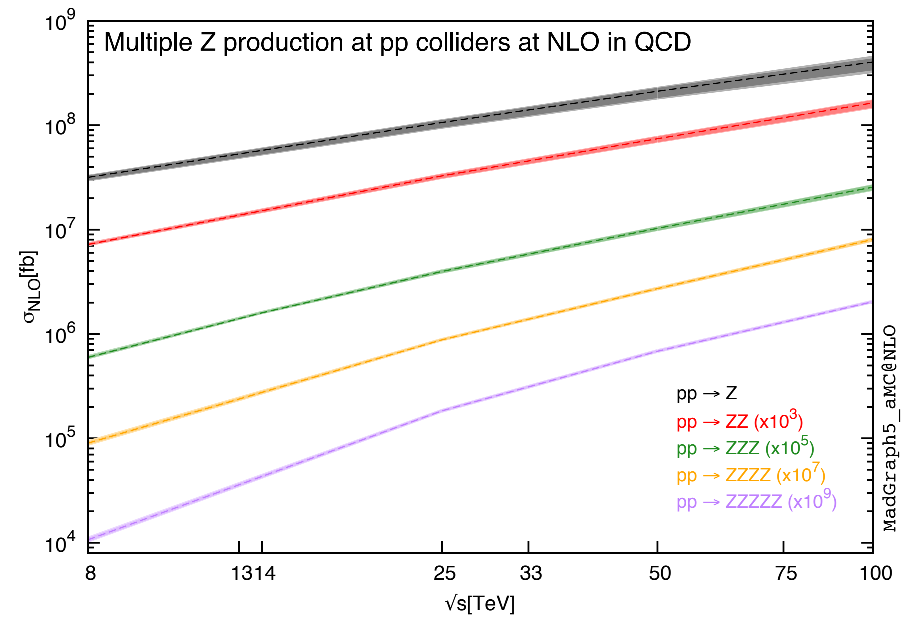
arXiv:1401.7340 [hep-ph]

NLO+PS

All results include scale and PDF uncertainties

→ See M. Zaro's talk

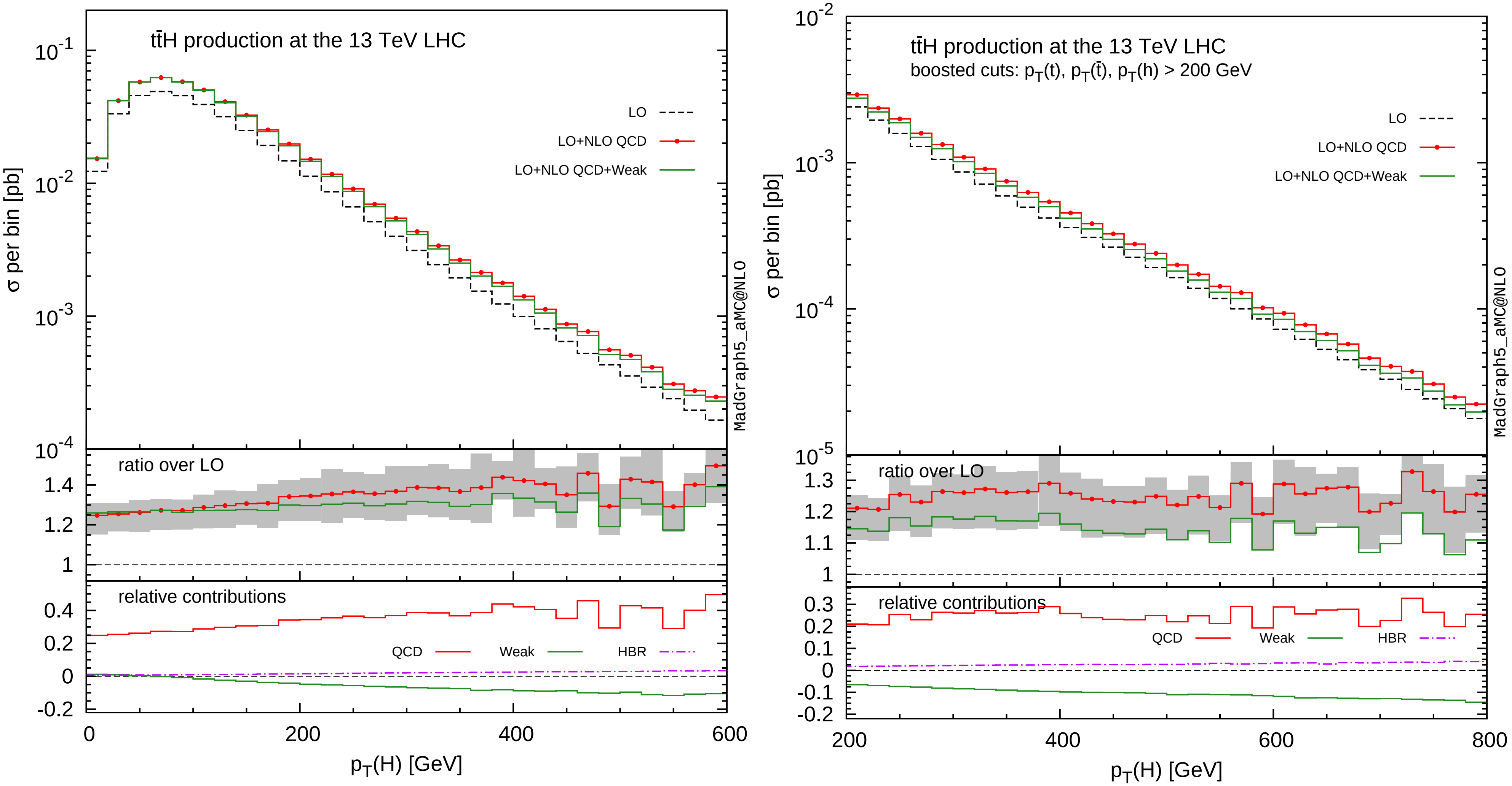




SM at NLO: thickness of lines is scale+PDF uncertainties

arXiv:1407.1623 [hep-ph] New!

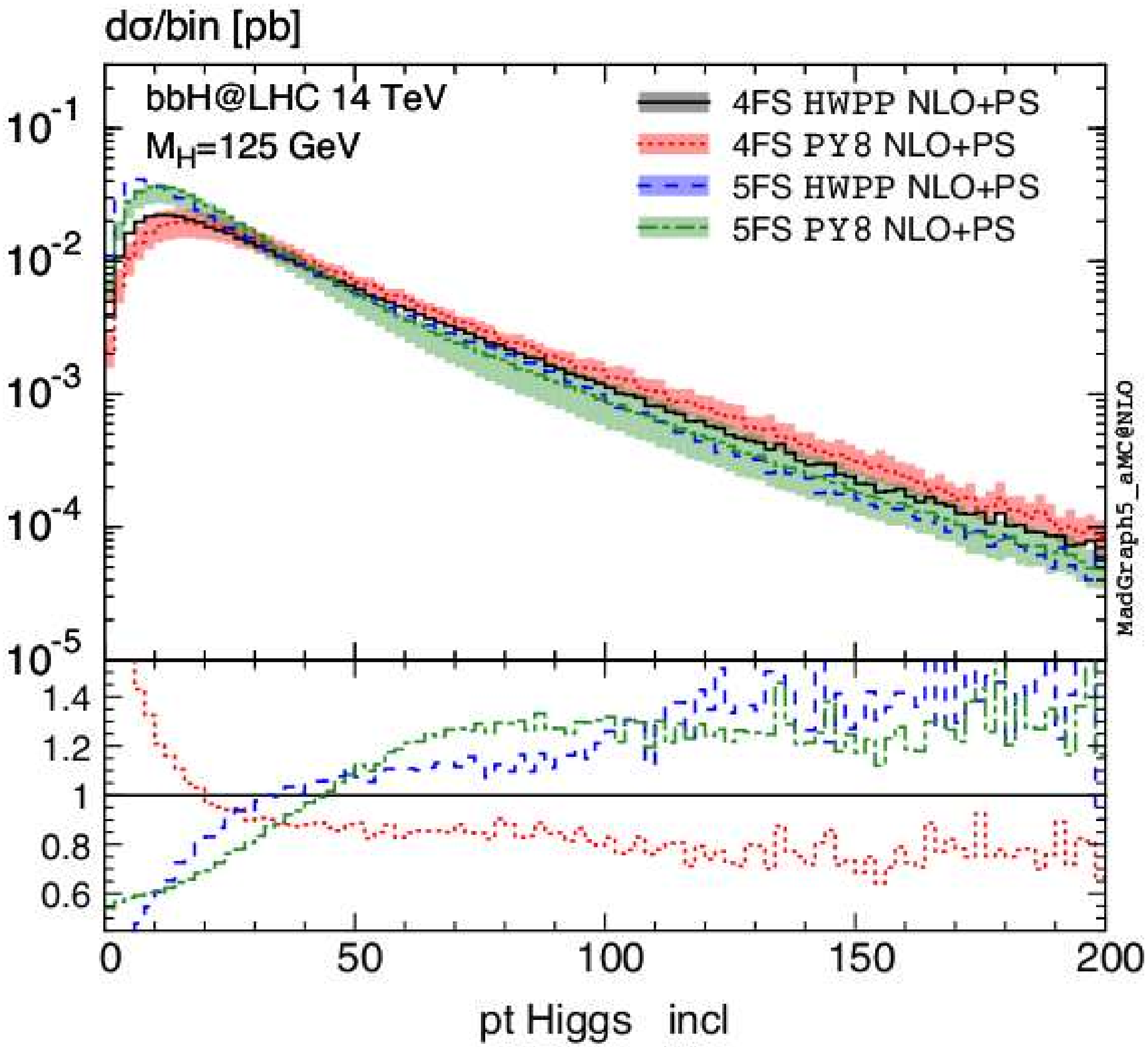
(Paolo Torrielli)



Weak (and QCD) NLO corrections to $t\bar{t}H$ production **New!**

arXiv:1407.0823 [hep-ph]

(SF, Hirschi, Pagani, Shao, Zaro)



$b\bar{b}H$ production at NLO+PS **New!**

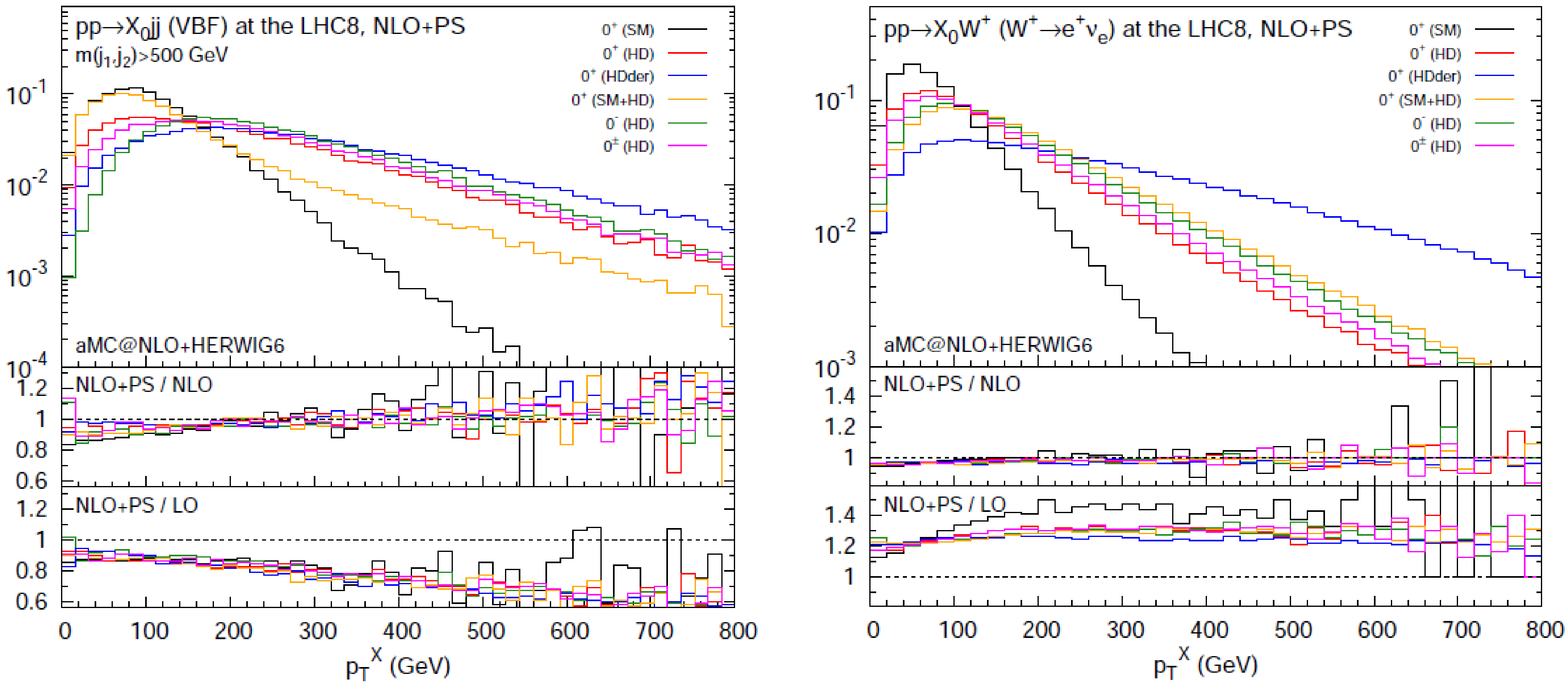
Wiesemann *etal*, in preparation

Take-home messages:

- Automation has enlarged the scope of NLO(+PS) results beyond imagination (*each* of the previous results used to be the outcome of *years* of work)

- We'll soon be able to compute any kind of corrections in any kind of theory, thanks to the automated construction of the relevant NLO specific building blocks – see in particular arXiv:1406.3030 (C. Degrande)

  E.g. SUSY in SUSY; QCD in light-Higgs EFTs $\longrightarrow$



p_T of a spin-0 state in VBF and W-associated production modes

arXiv:1311.1829 [hep-ph] (Maltoni, Mawatari, Zaro)

See also arXiv:1306.6464 ($gg \to X_J$), arXiv:1407.5089 ($gg \to X_0 jj$ and $t\bar{t}X_0$) New!

An aside, for the record:

- EFTs give the most general, systematically-improvable, way of studying Higgs characterisation in a model-independent manner

- They also show that *real* couplings are in general* perfectly sufficient to address any questions relevant to CP properties

* E.g. in a single-Higgs EFT below the EWSB scale, the only complex coupling is that of $HW^+_\mu \partial_\nu W^{-\mu\nu}$ (see 1306.6464)

NLO MERGING

NLO merging

Terminology

- An NLO *matching* procedure is MC@NLO or POWHEG
- An LO *merging* procedure is CKKW or MLM

Hence, with NLO merging I mean the extension of techniques such as CKKW or MLM to simulations whose individual results are accurate to NLO. There may thus exist different NLO mergings for the same matching strategy, and not only for different types of matching

Proposals

MEPS@NLO [Sherpa] (Hoeche, Krauss, Schonherr, Siegert + Gehrmann)
1207.5030, 1207.5031

FxFx [MadGraph5_aMC@NLO] (Frederix, SF) 1209.6215

Herwig++ (Plätzer) 1211.5467

Geneva (Alioli, Bauer, ...) 1211.7049

UNLOPS, NL^3 [Pythia8] (Lönnblad, Prestel) 1211.7278

The physics scope of these overlaps with that of
MiNLO (Hamilton, Nason, Zanderighi) 1206.3572

What do we expect?

Example: $gg \to H$

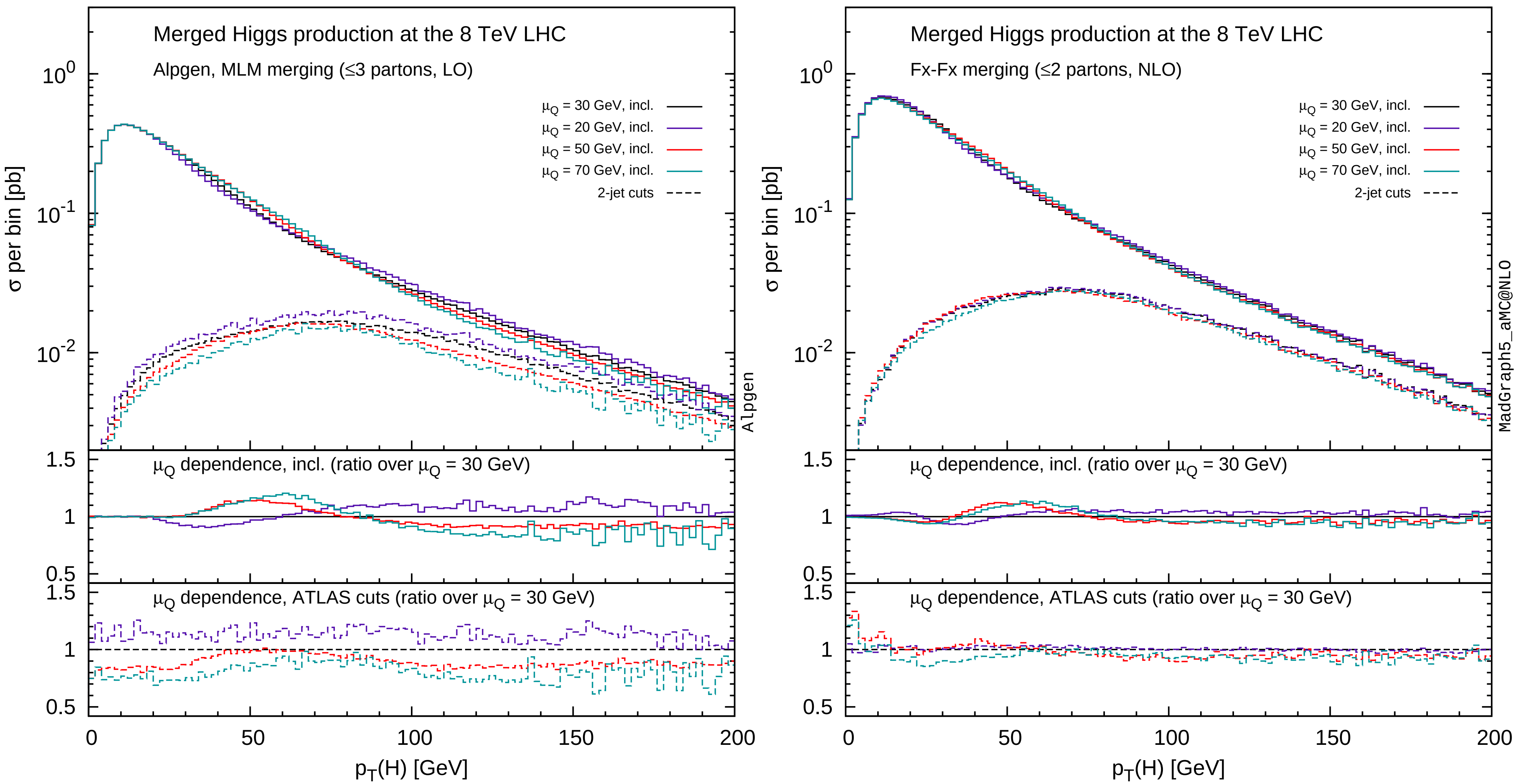
Merged samples (0-, 1-, and 2-parton) with $\mu_Q = 20$, 30, 50, and 70 GeV

FxFx (NLO) and Alpgen (LO, includes 3 partons)

Anti-k_T jets, $R = 0.4$, only those with $|\eta| \leq 5$ considered

- cuts$_1$ (aka 2-jet):
  at least two jets, both with $p_T \geq 25$ GeV
- cuts$_2$ (aka VBF-like):
  $M_{j_1 j_2} \geq 400$ GeV && $|\Delta y_{j_1 j_2}| \geq 2.8$ && cuts$_1$

Merging: LO ⟶ NLO



Left: LO (Alpgen). Right: NLO (FxFx in MadGraph5_aMC@NLO)

Happy? Not completely

- It has taken a long time to establish merging at the LO. The NLO case is much more difficult, and there are vast differences among the various proposals, which have *not* been properly assessed so far

- Things do break down, if one tries hard enough. This is an opportunity for improving both merging techniques and MCs

Take a look at what happens with VBF-like cuts $\longrightarrow$

Rates (pb)

MadGraph5_aMC@NLO and Alpgen

	$\mu_Q = 20$	$\mu_Q = 30$	$\mu_Q = 50$	$\mu_Q = 70$
no cuts	14.47 8.84	14.56 8.92	14.77 9.08	14.78 9.07
cuts_1	1.65 1.27	1.63 1.12	1.60 1.01	1.55 0.92
cuts_2	0.117 0.085	0.119 0.080	0.166 0.118	0.201 0.142

ME $\longleftarrow$ $\longrightarrow$ MC

Ratios $x(\mu_Q)/x(\mu_Q = 30)$

MadGraph5_aMC@NLO and Alpgen

	$\mu_Q = 20$	$\mu_Q = 30$	$\mu_Q = 50$	$\mu_Q = 70$
no cuts	0.994	1	1.014	1.014
	0.991	1	1.018	1.019
cuts$_1$	1.008	1	0.976	0.946
	1.132	1	0.905	0.816
cuts$_2$	0.982	1	1.389	1.685
	1.063	1	1.471	1.778

Read by rows (merging-scale dependence)

The I-don't-want-to-look-for-troubles attitude

Since $p_T^{(min)}(jet) = 25$ GeV, take $\mu_Q = 25 \pm 5$ GeV and see what happens:

- It works very well. Btw, NLO merging-scale dependence is 1.8% at most

But: we know that MC effects extend very far $(p_T \sim m_H/2)$.
Why should we blindly decide that we trust an ME description,
just because we are studying two-jet (VBF-like cuts) observables?

The treat-the-systematics-seriously attitude

Push μ_Q to $\mathcal{O}(m_H/2)$:

- Total cross sections are very stable (1.5%), and very close to the inclusive $\mathcal{O}(\alpha_S^3)$ one (in spite of FxFx not imposing unitarity)
- Rather consistent with Alpgen (scaling properties within 20% of each other)
- Even with cuts$_1$, μ_Q dependence is a mere 6%, down from the 18% of Alpgen (LO $\longrightarrow$ NLO)
- However, cuts$_2$ (68% in FxFx, 78% in Alpgen) seem to suggest that all is not well

Take-home messages:

- The majority of the tests performed so far are successful, but we have also uncovered a problem or two, whose solution is so far unclear (to me, at least...). Must do:
  - Systematic comparisons with data
  - Systematic comparisons of the different approaches

- A crucial point: going to NLO must not be used as an excuse to vary the merging scale in a range narrower than at the LO

The routine use of NLO-merging approaches by LHC experiments will be extremely important to establish or disprove them firmly

Conclusions

NLO+PS's are now widespread, and must be considered the default type of simulation in HEP

- The predictivity inherent to NLO computations is an asset. Thus, *all* theoretical uncertainties must be systematically studied

- Automation opens vast possibilities. Remember that it also implies that your favourite process might not have been explicitly mentioned anywhere, in spite of being perfectly feasible (and guaranteed to be correct)

- NLO merging techniques are a new frontier: validation efforts are needed, and will pay back

EXTRA SLIDES

Theory uncertainties: MC@NLO

Key point: the dependences on coupling constants, logarithms of scales, and PDFs is linear in the short-distance MC@NLO cross section

$\Longrightarrow$ Define scale- and PDF-independent coefficients, and use them to compute scale and PDF uncertainties by *reweighting*

This has zero CPU cost! All MadGraph5_aMC@NLO event samples include by default these reweighting coefficients (see 1110.4738)

- Note: this is at the short-distance cross section level. The interplay with choices made in the MC is an open issue, which is being studied (Webber, SF)

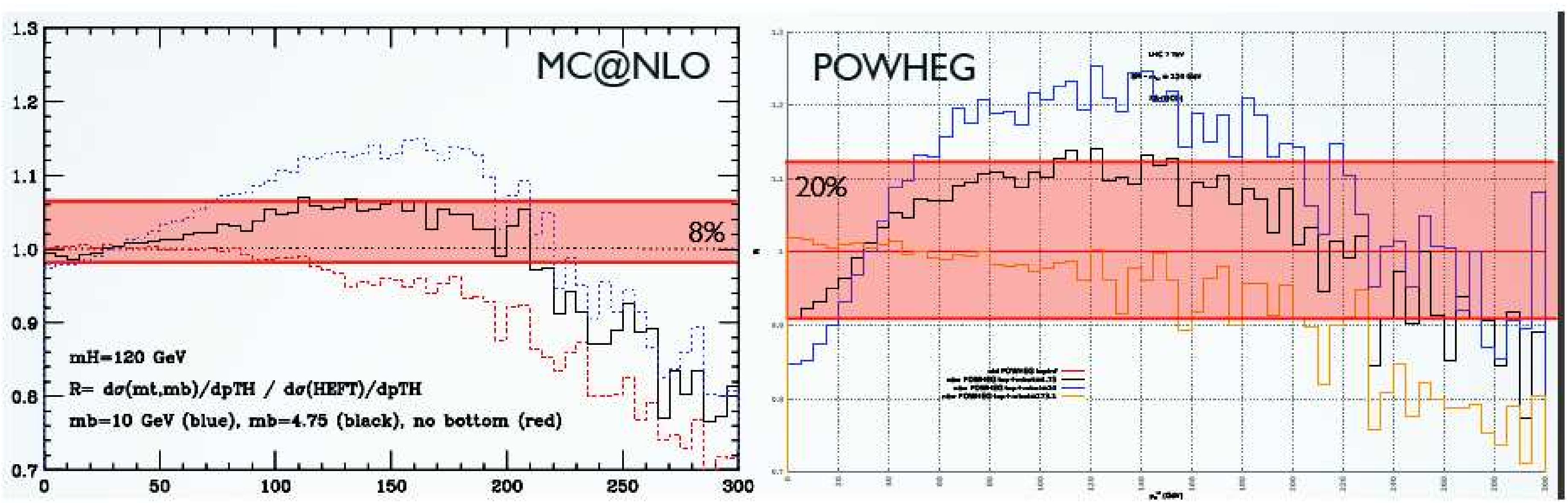
Theory uncertainties: POWHEG

- Cannot change scales in Δ_R without spoiling logarithmic accuracy
- Scale dependence of $\overline{\mathcal{M}}^{(b)}$ is standard. However, its role in the POWHEG formula implies that the shape of the first emission is independent of scales (i.e., $d\sigma/dp_T(H)$ for any $p_T(H) > 0$ has the same scale uncertainty as the total rate)
- The above is not correct if one uses the damp version (owing to $\mathcal{M}_F^{(r)}$). However, this exposes the fact that it is also necessary to study the systematics due to the choice of $F(p_T)$ (see $p_T(H)$ in $gg \to H$)

All this is being considered (Hamilton, Nason)

I don't know whether reweighting techniques are viable, and am not aware of general approaches to PDF systematics

Higgs p_T spectrum



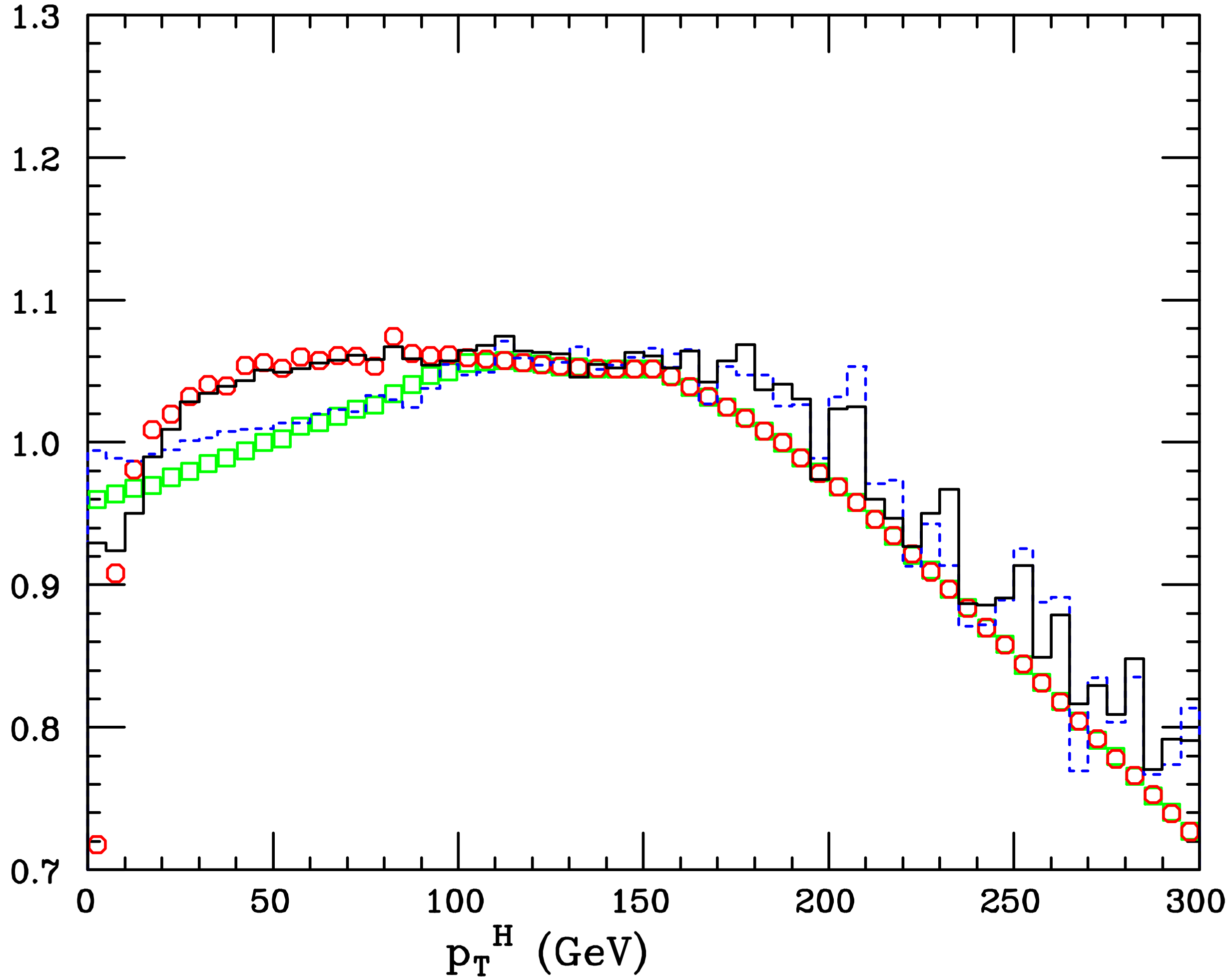
m_t and m_b effects, relative to HEFT, in $gg \to H^0$ at $\mathcal{O}(\alpha_S^3)$

MC@NLO v4.08

POWHEG 1111.2854 (Bagnaschi, Degrassi, Slavich, Vicini)

The two codes use the same matrix elements. Absolute normalization disregarded in this comparison

MC@NLO vs HRES



histograms: MC@NLO symbols: HRes

solid and circles: $Q_2 = \mathcal{O}(m_b)$ dashed and boxes: $Q_2 = \mathcal{O}(m_H)$

A proposal to treat quark-mass effects with POWHEG

- In the following identity the square bracket is a correction to the first, only-top, term because of the yukawa suppression of the bottom coupling

$$|\mathcal{M}(t+b)|^2 = |\mathcal{M}(t)|^2 + \left[|\mathcal{M}(t+b)|^2 - |\mathcal{M}(t)|^2\right]$$

- The first term contains the full top-quark squared amplitude;
  the square bracket contains the top-bottom interference and the bottom squared amplitude

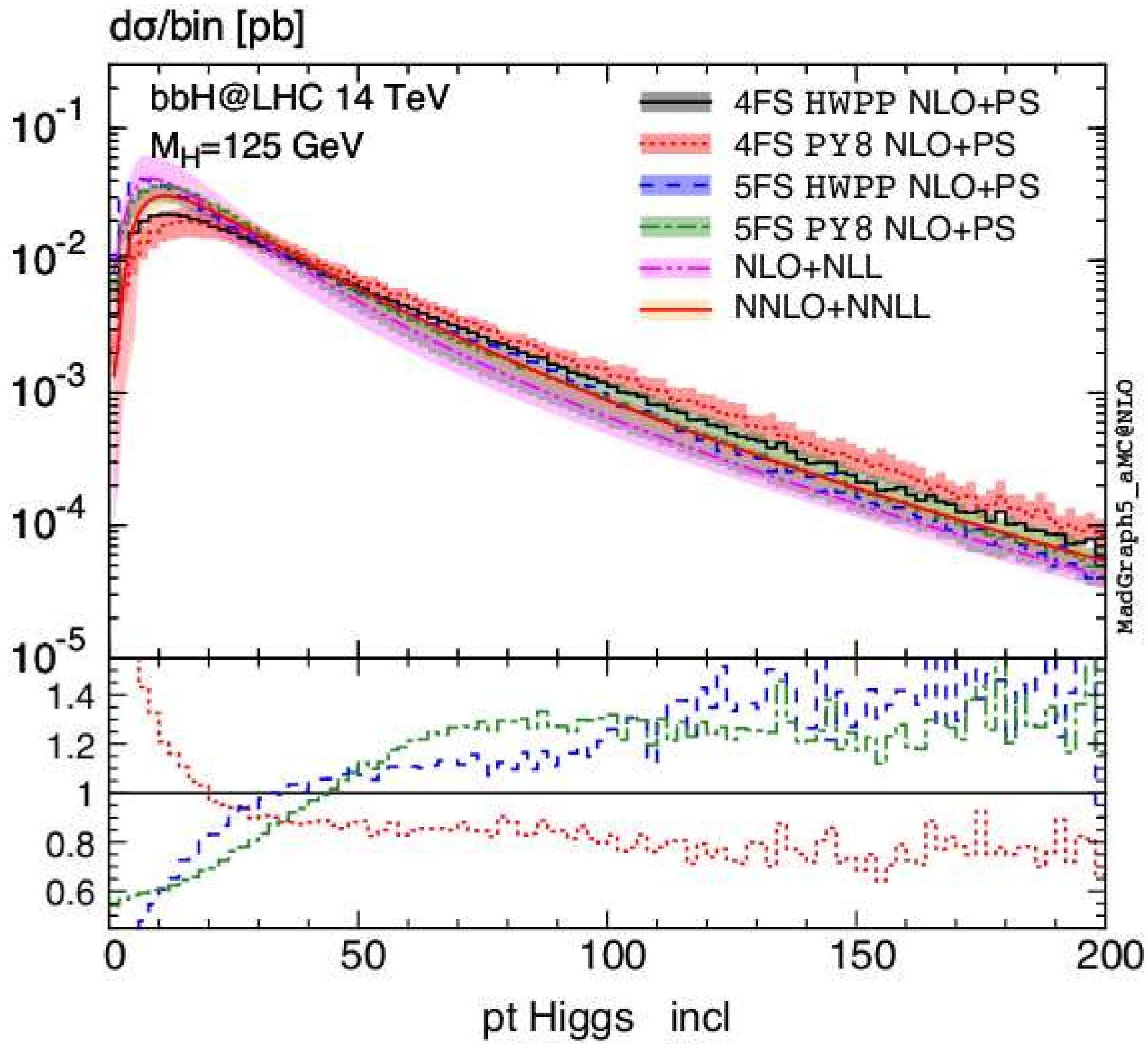
- The total cross section is independent of the choice of *h*
  → the total cross section, including quark-mass effects, can be written as

$$\sigma(t+b) = \sigma(t, h = m_H/1.2) + [\sigma(t+b, h = m_b) - \sigma(t, h = m_b)]$$

- Since the first term depends only on the top quark, a sensible choice is *h*=MH/1.2

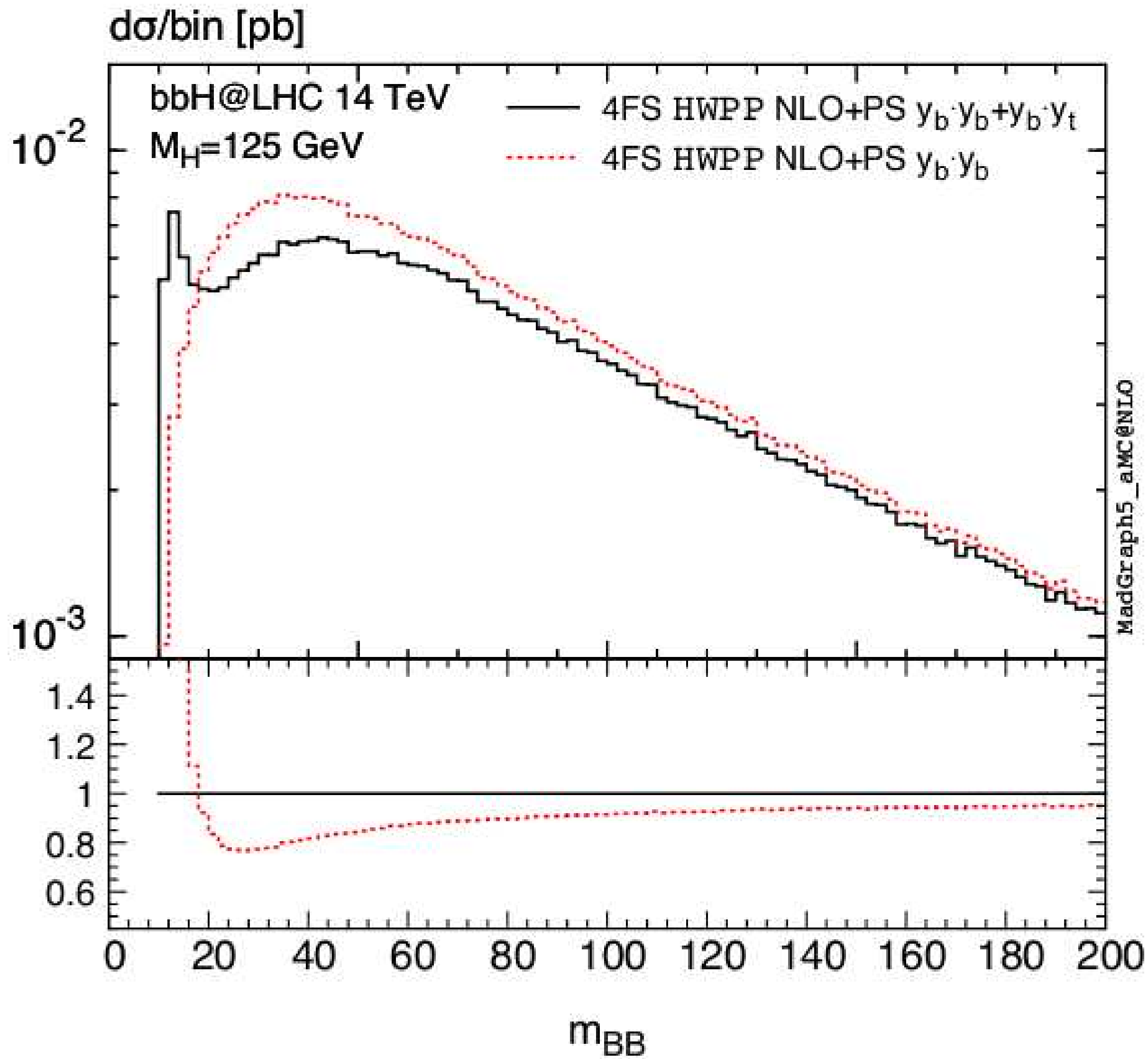
- Since the square bracket contains the top-bottom interference and the bottom squared amplitude, but no pure top-quark contribution, a sensible choice is *h*=mb

- We propose to use the above formula also for the differential distributions



$b\bar{b}H$ production at NLO+PS New!

Wiesemann *etal*, in preparation



$b\bar{b}H$ production at NLO+PS New!

Wiesemann *etal*, in preparation

FxFx merging (1209.6215)

- The i-parton sample receives contributions from the same matrix elements that enter the i-jet cross section at the NLO

- The i-parton cross section is basically the MC@NLO one, times a suitable combination of damping factors defined with a (smooth) function $D(\mu)$, which allow one to distinguish ME-dominated, MC-dominated, and intermediate regions

- $D(\mu)$ can also be chosen to be sharp, in which case

$$D(\mu) = \Theta\left(\mu_Q - \mu\right)$$

  with μ_Q the merging scale

- The above is further supplemented by a CKKW-like procedure