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Monte Carlos and NLO QCD

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Where we stand

	Good	*Bad*	*Users*
NLO	Hard emissions Total rates	Soft&coll emissions Hadronization No events	Theorists
MC	Soft&coll emissions Hadronization Outputs events	Hard emissions Total rates	Experimentalists

In other words: NLO $\bigcap$ MC $= \emptyset$

A formalism incorporating NLO *and* MC should combine their Good features, avoiding the Bad ones. However, the radical differences between the two approaches made QCDists wonder whether such a combination was possible

Motivations for matching NLO and MC

A formalism with all the Good features is certainly desirable, and its definition is a challenging theoretical problem. But, are there compelling physical motivations?

- It is not unlikely that new physics signals will emerge from counting experiments, which require firm control on SM signal and background simulations
- The high-energy regime of the Tevatron and the LHC implies the relevance of multi-jet, multi-scale processes, with large K-factors
- Standard MC's don't perform well in predicting multi-jet observables, and the practice of multiplying the results by inclusive K-factors is just wrong. This may lead to major errors in the strategies for searches
- Multi-scale processes are badly predicted by fixed-order computations. Results matching these computations with resummed ones are mandatory (a procedure largely successful at LEP)
- The hadronization procedure in NLO computations is extremely naive, and strictly speaking can be applied only at very large p_T's

Objectives

Our aim is to develop a practical method for combining existing parton shower MC programs with NLO perturbative calculations; the resulting object is called NLOwPS. Let's start with some *definitions*

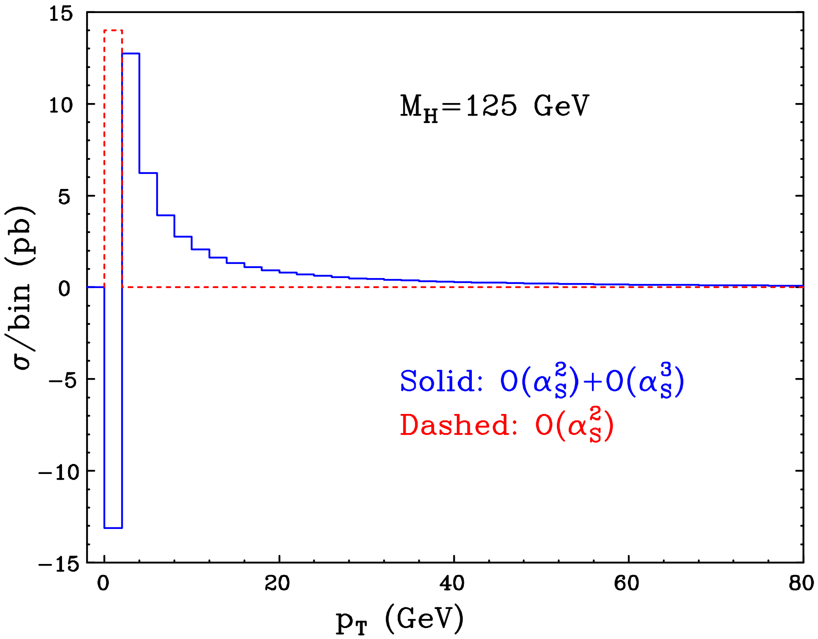
- Total rates are accurate to NLO
- Hard emissions are treated as in NLO computations
- Soft/collinear emissions are treated as in MC
- NLO results are recovered upon expansion of NLOwPS results in α_S. In other words: there is no double counting in NLOwPS
- The matching between hard- and soft/collinear-emission regions is smooth
- The output is a set of events, which are fully exclusive
- MC hadronization models are adopted

NLOwPS is not positive definite, and some events may have negative weights. From the user's point of view, it works just like an ordinary MC

Warning: a related, but different, procedure aims at incorporating multi-leg, real emission diagrams into MC's – virtual diagrams are thus not included

What does NLO mean?

Consider Higgs production:



$$\frac{d\sigma}{dp_T} = \left(A\alpha_S^2 + B\alpha_S^3\right)\delta(p_T) + C(p_T)\alpha_S^3$$

$$\int_{p_T^{min}}^{\infty} dp_T \frac{d\sigma}{dp_T} = \mathcal{C}_3\alpha_S^3, \qquad p_T^{min} > 0$$

$$= \mathcal{D}_2\alpha_S^2 + \mathcal{D}_3\alpha_S^3, \quad p_T^{min} = 0$$

$p_T^{min} > 0 \Rightarrow$ LO, $p_T^{min} = 0 \Rightarrow$ NLO

The answer depends on the observable, and even on the kinematic range considered.
So this definition cannot be adopted in the context of event generators

- N^{k}LO accuracy in event generators is defined by the number k of extra gluons (either virtual or real) wrt the LO contribution (hopefully we all agree on LO definition)

The actual NLOwPS's

- MC@NLO (Webber & SF; Nason, Webber & SF)
  Based on NLO subtraction method
  Formulated in general, interfaced to Herwig
  Processes implemented: $H_1 H_2 \longrightarrow$ W^+W^-, $W^\pm Z$, ZZ, $b\bar{b}$, $t\bar{t}$, H^0, $W^\pm$, Z/γ

- Φ-veto (Dobbs & Lefebvre)
  Based on NLO slicing method
  Avoids negative weights, at the price of double counting
  Processes implemented: $H_1 H_2 \longrightarrow$ Z, $W^\pm$

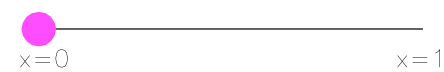
- GRACE_LLsub (Kurihara *et al*)
  Based on NLO hybrid slicing method, computes ME's numerically
  Double counts, unless the parton shower is not tuned
  Process implemented: $H_1 H_2 \longrightarrow$ Z

A proposal by Collins aims at including NLL effects in showers, but lacks gluon emission, so it is useless in QCD. Φ-veto is based on an old proposal by Baer&Reno; jets in DIS have been considered by Pötter&Schörner using a similar method. Soper&Krämer implemented $e^+e^- \to 3$ jets (but without a realistic MC)

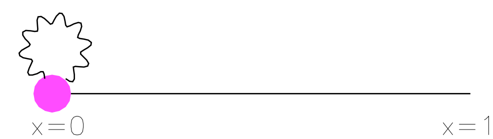
A simple way to understand NLOwPS

A system S moves along a line between 0 and 1. It can radiate "photons", whose energy we denote with x. S can undergo several further emissions; on the other hand, one photon cannot branch. Internal degrees of freedom of S are understood

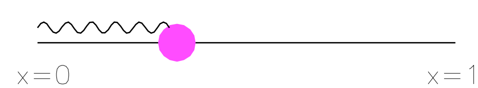
$$\left(\frac{d\sigma}{dx}\right)_B = B\delta(x) \qquad \longleftrightarrow$$



$$\left(\frac{d\sigma}{dx}\right)_V = \alpha_S \left(\frac{B}{2\epsilon} + V\right)\delta(x) \qquad \longleftrightarrow$$



$$\left(\frac{d\sigma}{dx}\right)_R = \alpha_S \frac{R(x)}{x} \qquad \longleftrightarrow$$



where $\lim_{x\to 0} R(x) = B$ as in QCD. An NLO prediction:

$$\frac{d\sigma}{dO} = \lim_{\epsilon\to 0}\int_0^1 dx x^{-2\epsilon}\delta(O - O(S,x))\left[\left(\frac{d\sigma}{dx}\right)_B + \left(\frac{d\sigma}{dx}\right)_V + \left(\frac{d\sigma}{dx}\right)_R\right]$$

with $\lim_{x\to 0} O(S,x) = O(S,0)$ (infrared safeness). Note the kinematics:

B&V $\Longrightarrow$ $O(S,0)$, R $\Longrightarrow$ $O(S,x)$

The computation of the NLO cross section I

■ *SLICING*

$$\left(\frac{d\sigma}{dO}\right)_{NLOslice} = \int_{\delta}^{1} dx \left\{ \delta(O - O(S,x)) \frac{\alpha_S R(x)}{x} \right.$$

$$\left. + \delta(O - O(S,0)) \Big[B + \alpha_S \left(B \log \delta + V \right) \Big] \right\}$$

■ *SUBTRACTION*

$$\left(\frac{d\sigma}{dO}\right)_{NLOsubt} = \int_{0}^{1} dx \left\{ \delta(O - O(S,x)) \frac{\alpha_S R(x)}{x} \right.$$

$$\left. + \delta(O - O(S,0)) \left(B + \alpha_S V - \frac{\alpha_S B}{x} \right) \right\}$$

B&V $\Longrightarrow O(S,0)$, R $\Longrightarrow O(S,x)$

The computation of the NLO cross section II

$$\left(\frac{d\sigma}{dO}\right)_{NLOsubt} = \int_0^1 dx \left\{ \delta(O - O(S,x)) \frac{\alpha_S R(x)}{x} + \delta(O - O(S,0)) \left(B + \alpha_S V - \frac{\alpha_S B}{x} \right) \right\}$$

Upon integration in x, the bin of $O(S,x)$ gets a weight

$$w_{\mathbb{H}}(x) = \frac{\alpha_S R(x)}{x}$$

and the bin of $O(S,0)$ gets a weight

$$w_{\mathbb{S}}(x) = B + \alpha_S V - \frac{\alpha_S B}{x}$$

The divergence of $w_{\mathbb{H}}(x)$ and $w_{\mathbb{S}}(x)$ for $x \to 0$ is the reason for:

1) numerical instabilities
2) the impossibility of getting unweighted events in NLO computations

The toy MC

The system can undergo an arbitrary number of emissions, with probability controlled by the Sudakov form factor

$$\Delta(x_1, x_2) = \exp\left[-\alpha_S \int_{x_1}^{x_2} dz \frac{Q(z)}{z}\right]$$

i.e., the probability that no photon be emitted with energy $x_1 < x < x_2$. The function $Q(z)$ parametrizes beyond-LL effects, with

$$0 \leq Q(z) \leq 1, \quad \lim_{z \to 0} Q(z) = 1$$

The Born cross section

$$\left(\frac{d\sigma}{dx}\right)_B = B\delta(x)$$

gives the overall normalization (B) and initial condition ($(S, 0)$) for the shower. Apart from the trivial normalization, this can be formally embedded in the generating functional (i.e., the history of all possible showers)

$$\boxed{\mathcal{F}_{\text{MC}}(S, 0)}$$

NLO $\oplus$ MC $\longrightarrow$ NLOwPS?

Naive first try: use the NLO kinematic configurations as initial conditions for showers, rather than for filling the histograms

- ♦ $\delta(O - O(S,0)) \longrightarrow$ start the MC with 0 emissions: $\mathcal{F}_{\mathrm{MC}}(S,0)$
- ♦ $\delta(O - O(S,x)) \longrightarrow$ start the MC with 1 emission at x: $\mathcal{F}_{\mathrm{MC}}(S,x)$

$$\mathcal{F}_{\mathrm{naive}} = \int_0^1 dx \left[\mathcal{F}_{\mathrm{MC}}(S,x) \frac{\alpha_S R(x)}{x} + \mathcal{F}_{\mathrm{MC}}(S,0) \left(B + \alpha_S V - \frac{\alpha_S B}{x} \right) \right]$$

It doesn't work:

- Cancellations between (S,x) and $(S,0)$ contributions occur after the shower: hopeless from the practical point of view; and, unweighting is still impossible
- $(d\sigma/dO)_{naive} - (d\sigma/dO)_{NLO} = \mathcal{O}(\alpha_S)$. In words: double counting

The problem is a fundamental one: KLN cancellation is achieved in standard MC's through unitarity, and embedded in Sudakovs. This is no longer possible: IR singularities do appear in hard ME's

MC@NLO: modified subtraction I

Get rid of the MC $\mathcal{O}(\alpha_S)$ contributions by an extra subtraction of $\mathcal{O}(\alpha_S)$

$$\mathcal{F}_{\text{MC@NLO}} = \int_0^1 dx \left[\mathcal{F}_{\text{MC}}(S,x) \frac{\alpha_S [R(x) - BQ(x)]}{x} \right. \\ \left. + \mathcal{F}_{\text{MC}}(S,0) \left(B + \alpha_S V + \frac{\alpha_S B[Q(x) - 1]}{x} \right) \right]$$

where the two (one for branching, one for no-branching probability) new terms are sensibly chosen:

$$\left(\frac{d\sigma}{dx} \right)_{MC} = \alpha_S B \frac{Q(x)}{x} + \mathcal{O}(\alpha_S^2)$$

$Q(x)$ is MC-dependent (i.e., Pythia's and Herwig's differ), but $Q(x) \rightarrow 1$ for $x \rightarrow 0$ always holds

By explicit computation, $(d\sigma/dO)_{MC@NLO} - (d\sigma/dO)_{NLO} = \mathcal{O}(\alpha_S^2)$, and therefore there is no double counting

Furthermore $\longrightarrow$

MC@NLO: modified subtraction II

Let's look at the weights of $\mathcal{F}_{\text{MC}}(S, x)$ and $\mathcal{F}_{\text{MC}}(S, 0)$

$$w_{\mathbb{H}}(x) = \frac{\alpha_S [R(x) - BQ(x)]}{x}$$

$$w_{\mathbb{S}}(x) = B + \alpha_S V + \frac{\alpha_S B[Q(x) - 1]}{x}$$

They don't diverge any longer for $x \to 0$

The MC provides local, observable-independent, counterterms $\Longrightarrow$ greater numerical stability, unweighting possible

MC@NLO can thus be minimally seen as a way to stabilize NLO computations, through the construction of a simplified MC whose only aim is to furnish the local counterterms. In this sense, the generalization to NNLO should not be too difficult

Modified subtraction in QCD

Strategy: Take the toy model seriously, and literally translate it in QCD language

$$\mathcal{F}_{\text{MC@NLO}} = \sum_{ab} \int dx_1\, dx_2\, d\phi_3\, f_a(x_1) f_b(x_2)$$
$$\Big[\mathcal{F}_{\text{MC}}^{(2\to3)} \left(\mathcal{M}_{ab}^{(h)}(x_1,x_2,\phi_3) - \mathcal{M}_{ab}^{(\text{MC})}(x_1,x_2,\phi_3)\right) +$$
$$\mathcal{F}_{\text{MC}}^{(2\to2)} \left(\mathcal{M}_{ab}^{(b,v,c)}(x_1,x_2,\phi_2) - \mathcal{M}_{ab}^{(c.t.)}(x_1,x_2,\phi_3) + \mathcal{M}_{ab}^{(\text{MC})}(x_1,x_2,\phi_3)\right)\Big]$$

Since it is literal...

$$\frac{\alpha_S R(x)}{x} \leftrightarrow \mathcal{M}_{ab}^{(h)}, \qquad \frac{\alpha_S BQ(x)}{x} \leftrightarrow \mathcal{M}_{ab}^{(\text{MC})}$$

it works only if $\mathcal{M}_{ab}^{(\text{MC})}$ is a local counterterm of $\mathcal{M}_{ab}^{(h)}$. This is not the case: large-angle soft gluon emission in MC's is not described by eikonals

Fortunately, the problem is not a serious one: we can still use existing MC's. Formally, some observables will get extra power-suppressed contributions; practically, the effects are invisible

What's the problem with the soft limit?

From perturbative computations, we expect the following formula to hold

$$d\sigma_{2\to 3} \quad \xrightarrow{E\to 0} \quad \frac{\alpha_S}{E^2}\frac{1}{1-\cos^2\theta}d\sigma_{2\to 2}$$

Using the MC (HERWIG) showering variables, we find instead

$$d\sigma_{2\to 3} \quad \xrightarrow{E\to 0} \quad \frac{\alpha_S}{E^2}\left[\frac{2\Theta(\cos\theta > -1/3)}{(1-\cos\theta)(3+\cos\theta)} + \frac{2\Theta(\cos\theta < 1/3)}{(1+\cos\theta)(3-\cos\theta)}\right] d\sigma_{2\to 2}$$

MC's are not designed to produce fixed-order results. As such, the initial conditions for the showers are chosen in order to maximize the efficiency, and the coverage of the phase space. However, it is legitimate to ask why MC's can describe physics, and still disagree with QCD

$$\int_{-1+\varepsilon}^{1-\varepsilon} d\cos\theta \left[\frac{2\Theta(\cos\theta > -1/3)}{(1-\cos\theta)(3+\cos\theta)} + \frac{2\Theta(\cos\theta < 1/3)}{(1+\cos\theta)(3-\cos\theta)} - \frac{1}{1-\cos^2\theta}\right] \quad \xrightarrow{\varepsilon\to 0} \quad 0$$

This equation is the answer: the total amount of "soft" energy given by the MC is in agreement with QCD. Physical observables must be independent of the angular distributions of soft gluons (beware of non-global logs)

MC@NLO: summary

1. Choose your favourite MC (Herwig, Pythia), and compute analytically the "NLO cross section", i.e., the first emission. This is an observable-independent, process-independent procedure, which is done once and for all

2. Combine the LO+NLO matrix elements of the process to be implemented according to the universal, observable-independent, subtraction-based formalism of SF, Kunszt, Signer for cancelling IR divergences. All counterterm, virtual, and LO contributions must have an unique kinematics (achieved through a projection)

3. Add and subtract the MC counterterms, computed in step 1, to the quantity computed in step 2. The resulting expression allows to generate the hard kinematic configurations, which are eventually fed into the MC showers as initial conditions

Some of these features are shared with multi-leg generators, implemented according to CKKW prescription: however, NLOwPS's don't have any dependence upon unphysical parameters

NLOwPS: Φ-veto

Exploit a proposal by Baer&Reno to get rid of the soft/collinear configurations:

$$B + \alpha_S \left(B \log \delta_0 + V \right) = 0 \quad \Longrightarrow \quad \delta_0 = \exp\Big[- \left(B + \alpha_S V \right) / \alpha_S B \Big]$$

Another parameter $\delta_{PS} > \delta_0$ separates the shower region from the hard region (Pötter, Schörner, Dobbs)

$$\mathcal{F}_{\Phi_{\text{veto}}} = \alpha_S \int_{\delta_{PS}}^{1} dx\, \mathcal{F}_{\text{MC}}(S, x) \frac{R(x)}{x} + \alpha_S\, \mathcal{F}_{\text{MC}}(S, 0) \int_{\delta_0}^{\delta_{PS}} dx\, \frac{R(x)}{x}$$

\+ *Only positive weights*

\+ *Doesn't need to know details of MC implementation*

– *Double counting for $x < \delta_{PS}$, and discontinuity at $x = \delta_{PS}$ imply dependence upon δ_{PS}, which is hidden by integration over Bjorken x's*

– *Strictly speaking, the (perturbative) result is non-perturbative, since $\delta_0 \sim \exp(-1/\alpha_S)$*

- Applied to: Z, $W^{\pm}$ production

NLOwPS: GRACE_LLsub

Partition the phase space as in standard slicing, but subtract the MC contribution from the hard region:

$$\mathcal{F}_{\mathrm{GRACE}} = \alpha_S \int_{\delta}^{1} dx\, \mathcal{F}_{\mathrm{MC}}(S,x) \frac{R(x) - B}{x} + \mathcal{F}_{\mathrm{MC}}(S,0)\,(B + \alpha_S V)$$

This formally coincides with MC@NLO, provided that

$$\delta \longrightarrow 0\,, \qquad Q(x) \equiv 1$$

The second condition cannot, however, be imposed: it must naturally result from the MC implementation

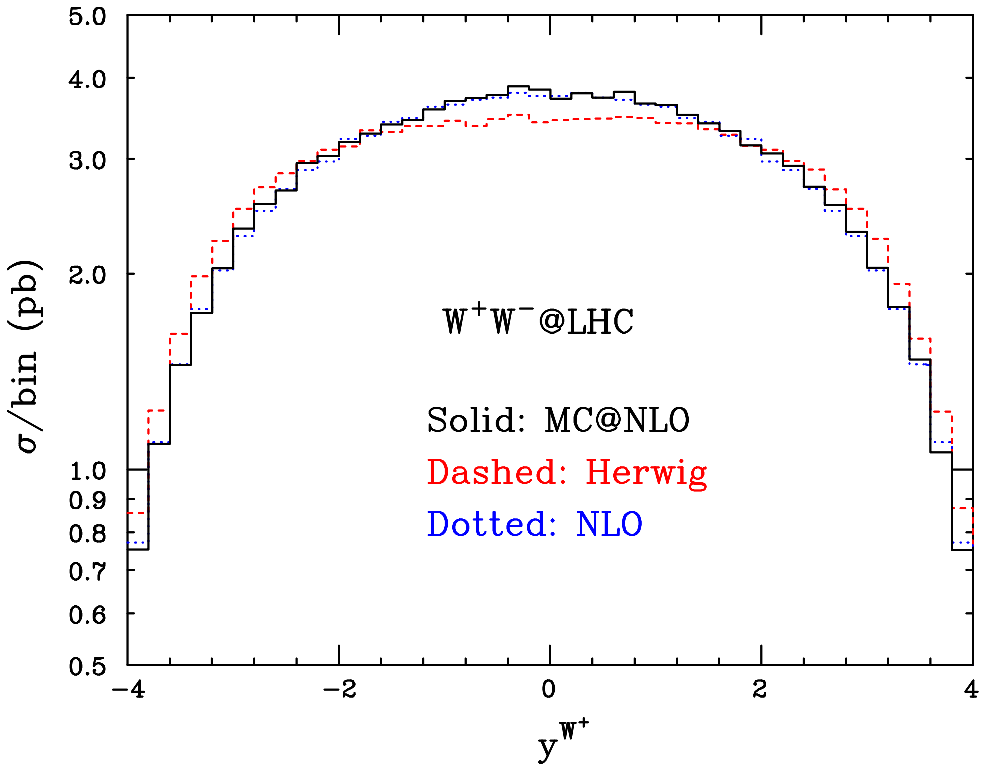
+ *All matrix elements generated numerically*

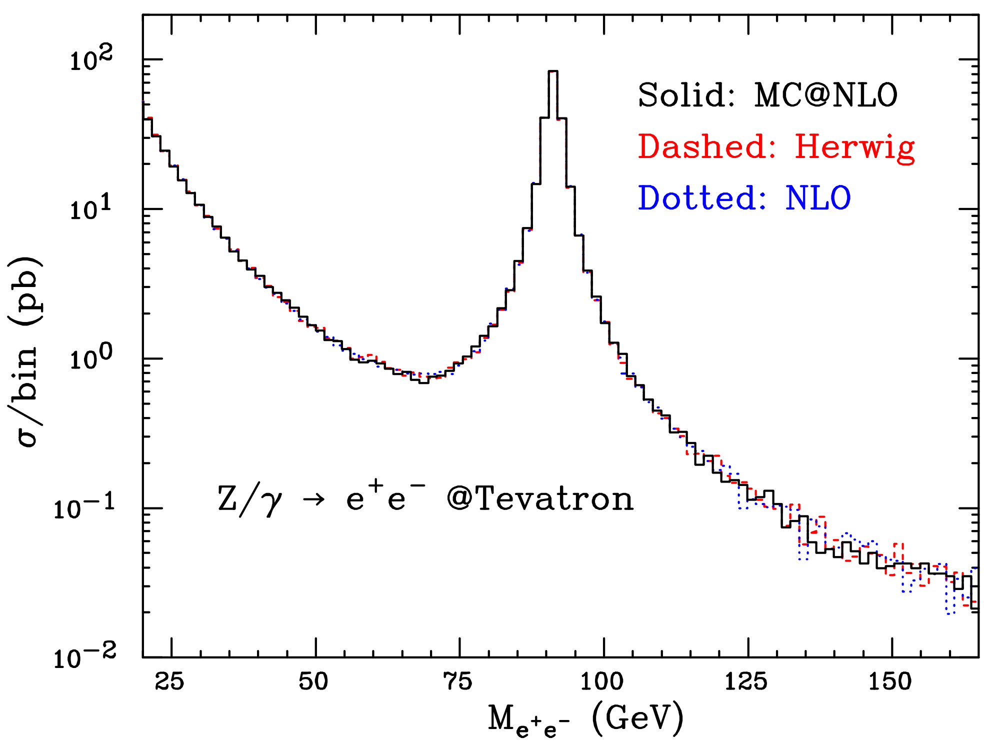
– *Double counting if $Q(x)$ is not tuned*

– *Tuning $Q(x)$ implies the construction of an ad-hoc MC*

- Applied to: Z production

The first check: MC@NLO $\simeq$ NLO





NLO is OK for these observables

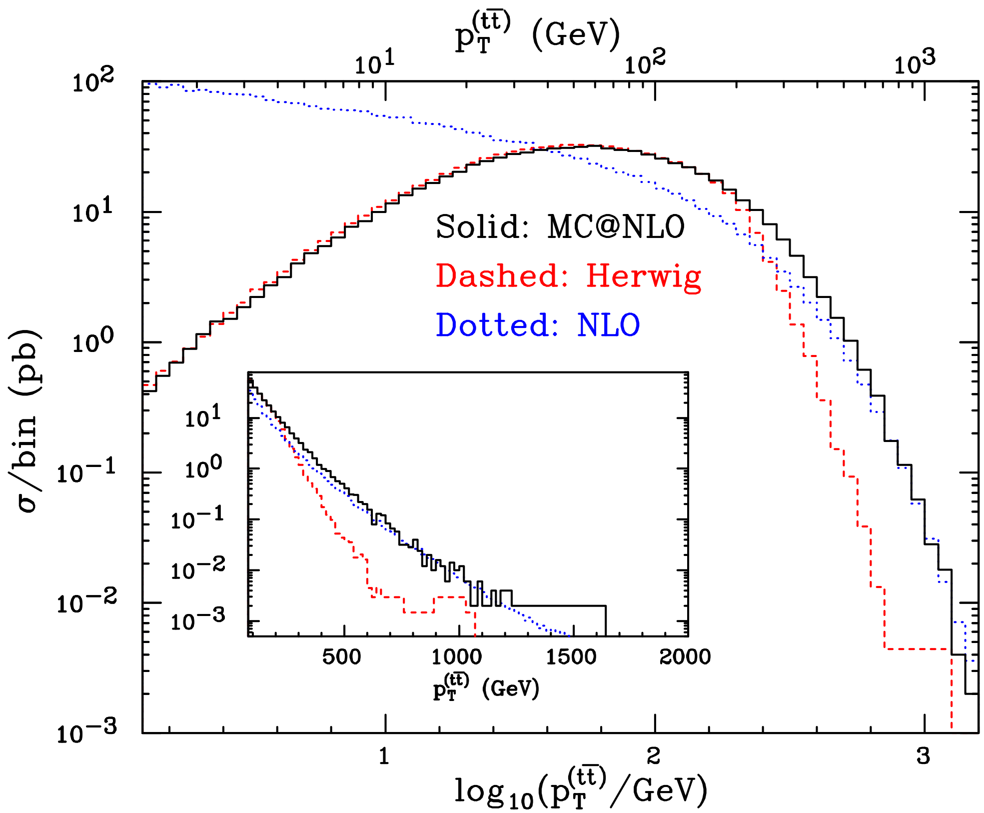
MC@NLO outputs a realistic final state, which matters when full detector simulation is included

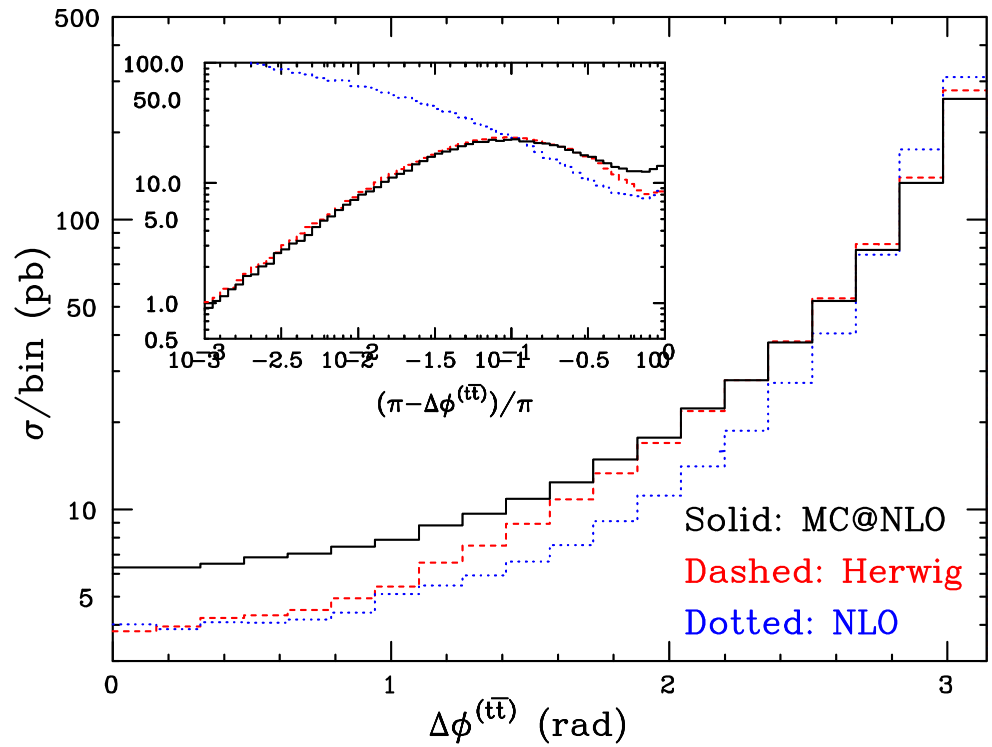
Solid: MC@NLO

Dashed: HERWIG$\times \frac{\sigma_{NLO}}{\sigma_{LO}}$

Dotted: NLO

A highly non-trivial check: $t\bar{t}$ at the LHC





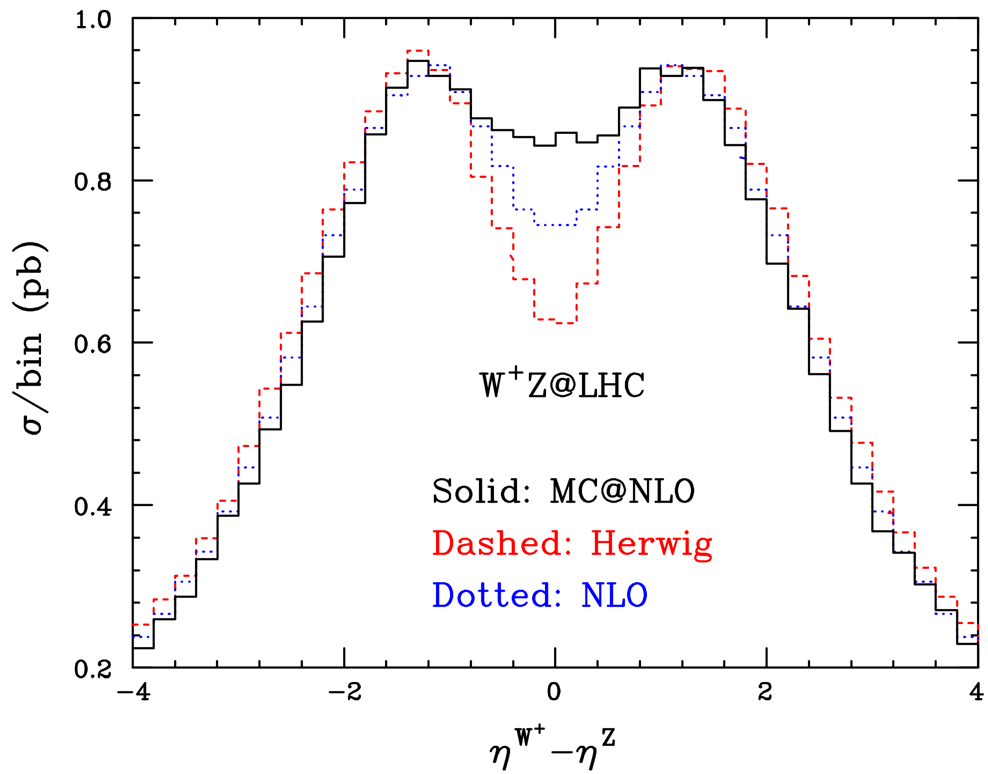
These correlations are problematic: soft and hard emissions are both relevant. MC@NLO does well, resumming large logarithms, and yet handling large-scale physics correctly

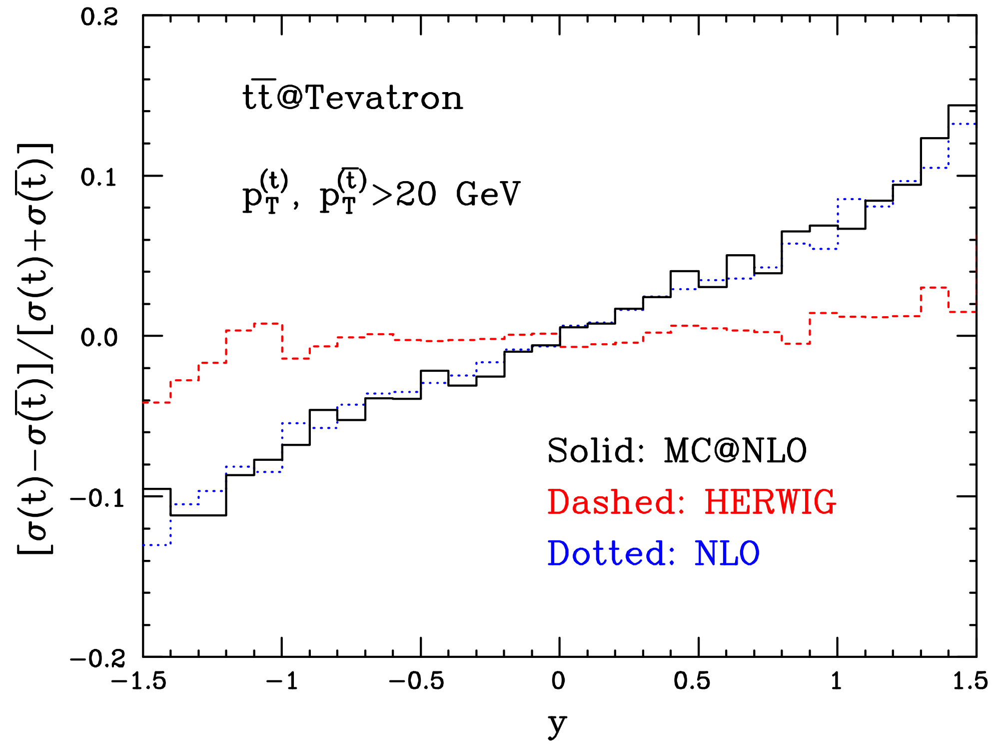
Solid: MC@NLO

Dashed: HERWIG$\times\frac{\sigma_{NLO}}{\sigma_{LO}}$

Dotted: NLO

New features in MC's





Radiation zero is further filled by MC@NLO

$t\bar{t}$ asymmetry is absent at the Born level, and thus also in standard MC's

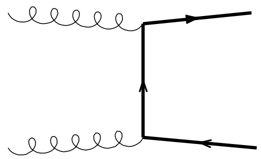
Solid: MC@NLO

Dashed: HERWIG

Dotted: NLO

Bottom production is much nastier than top

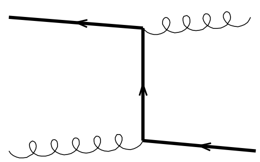
MC rule: if we aim to study any physical system, we start by producing it in the hard process $\Longrightarrow$



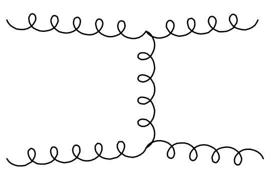
Flavour CReation

This is going to underestimate the rate by a factor of 4 (which is not so important), and to miss key kinematic features (which is crucial – see R. Field)

So break the rule and add other hard processes



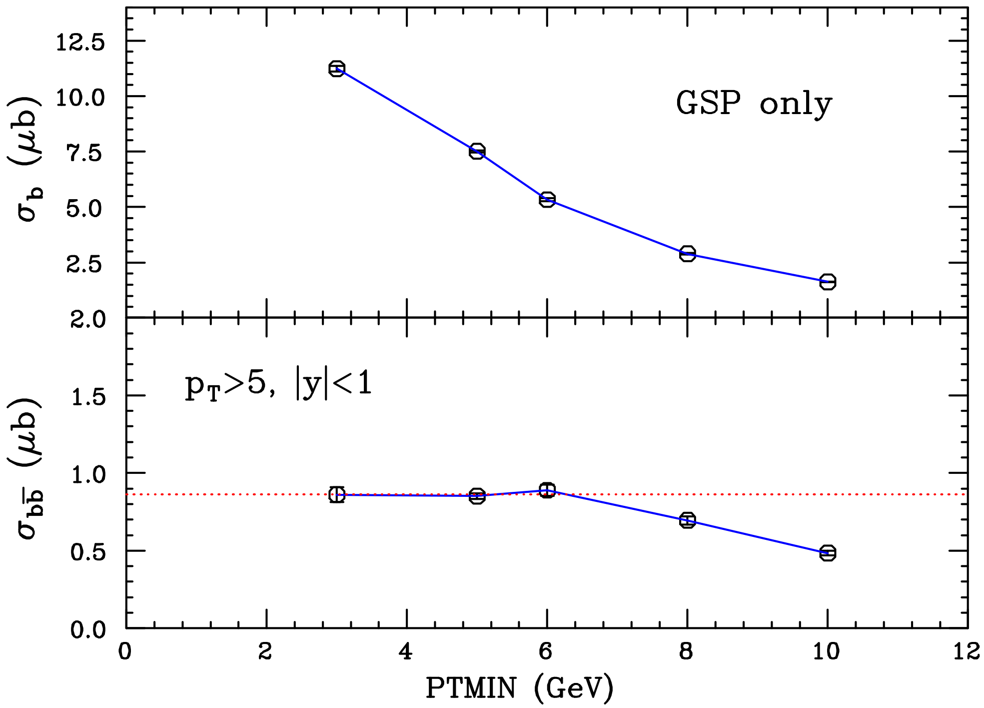
Flavour EXcitation

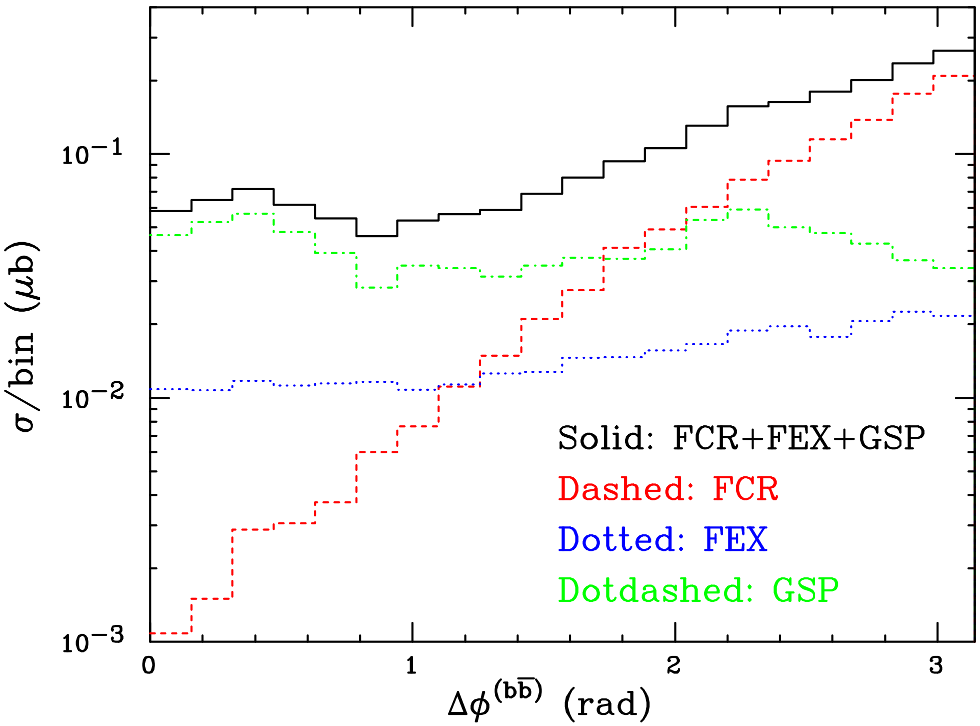


Gluon SPlitting

- In FEX, the missing b or $\bar{b}$ results from initial-state radiation. A cutoff PTMIN avoids divergences in the matrix element
- In GSP, the b and $\bar{b}$ result from final-state gluon splitting. PTMIN is again necessary to obtain finite results

b production with HERWIG



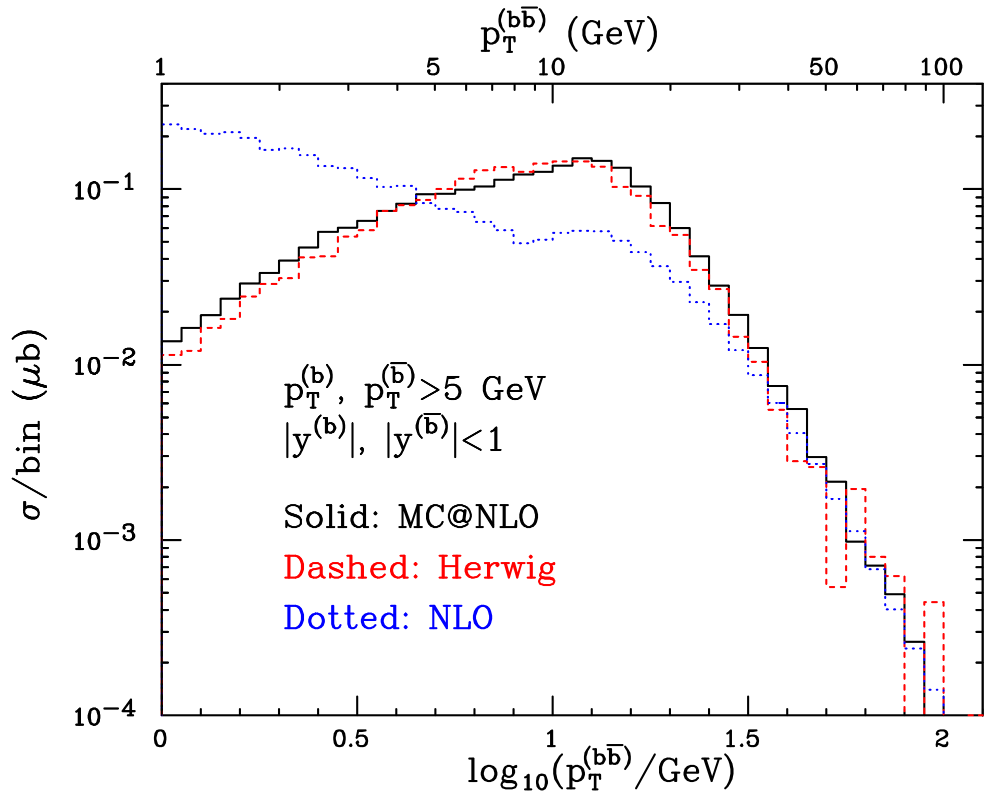


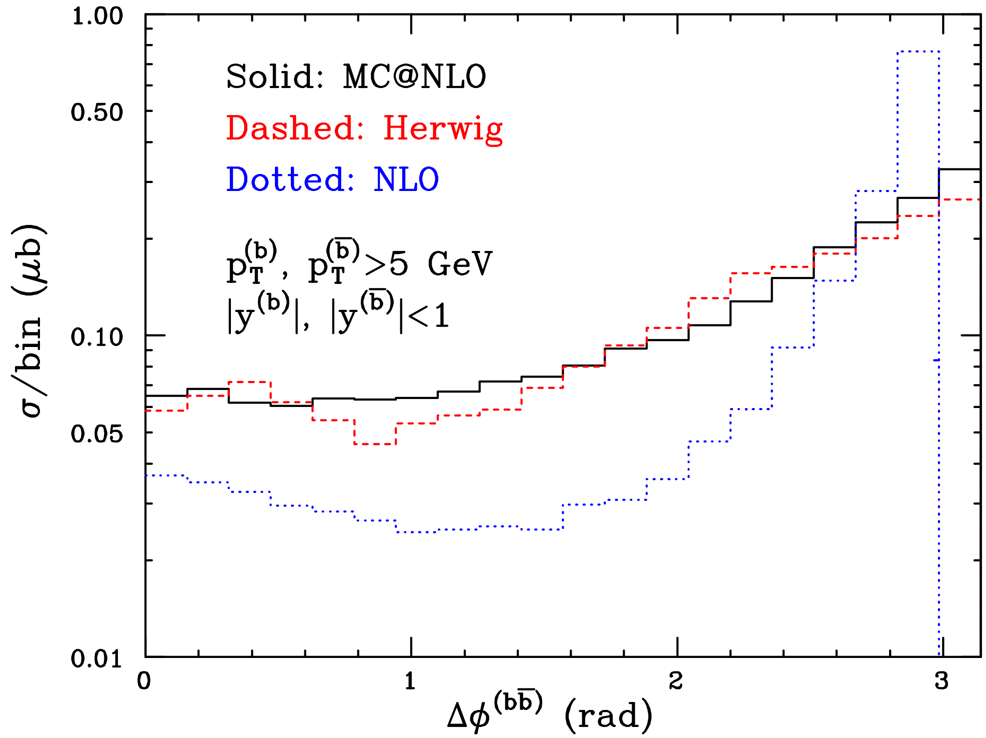
- The PTMIN dependence is worrisome in the case of single-inclusive observables
- FCR, FEX and GSP are complementary, and all must be generated
- GSP efficiency is extremely poor: 10^{-4} within cuts for correlations

Reliability and efficiency rapidly degrade for smaller p_T cuts. In FEX, the dependence on bottom PDF is problematic. No MC can work for $p_T \simeq 0$

All these problems are avoided with MC@NLO

$b\bar{b}$ correlations with MC@NLO





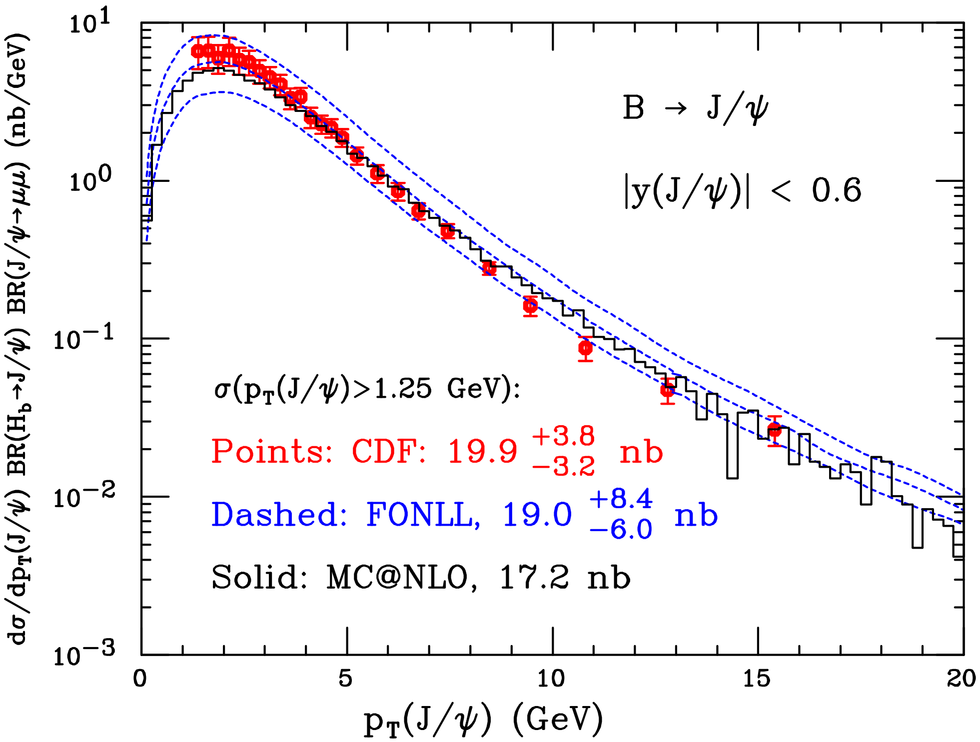
HERWIG does surprisingly well, but needs quite a lot of CPU (14 millions events – 1 million for MC@NLO). The hard emission effects are huge for b production, and cannot be neglected

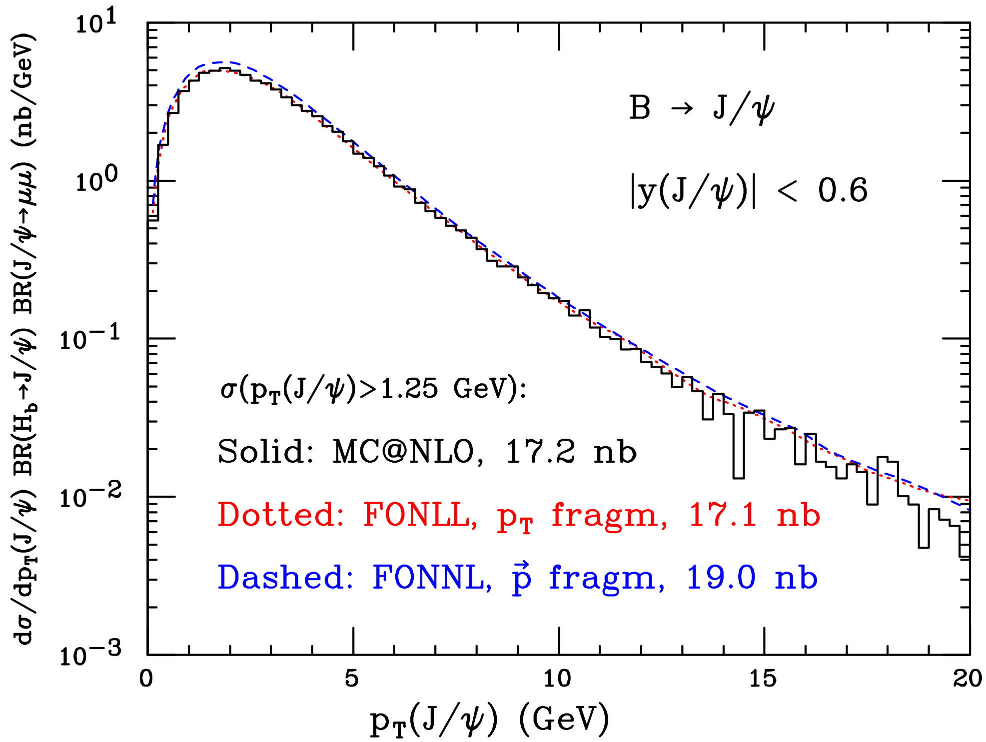
Solid: MC@NLO

Dashed: HERWIG

Dotted: NLO

Single-inclusive b at the Tevatron

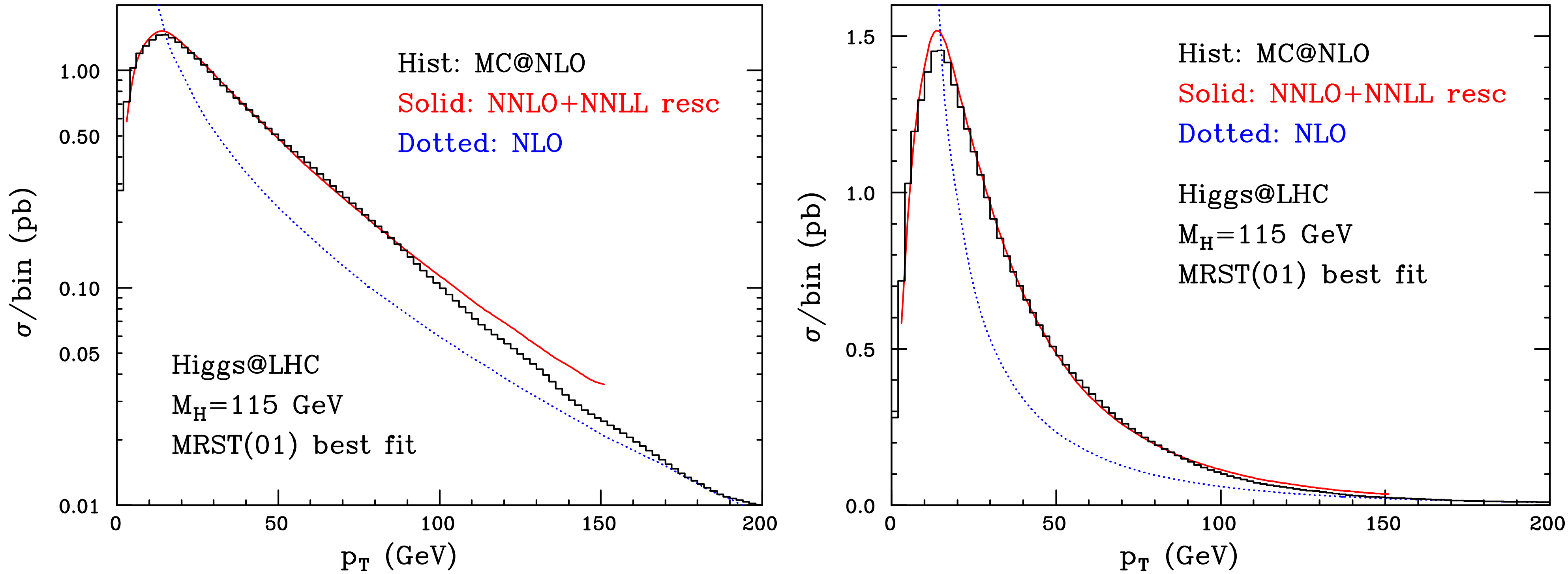




No significant discrepancy with data

- No PTMIN dependence in MC@NLO $\Longrightarrow$ solid predictions down to $p_T = 0$, no "perturbative-parameter tuning"
- Full agreement with NLL+NLO computation (FONLL, Cacciari&Nason), if the large dependence (at small p_T) on the hadronization scheme of the latter is taken into account

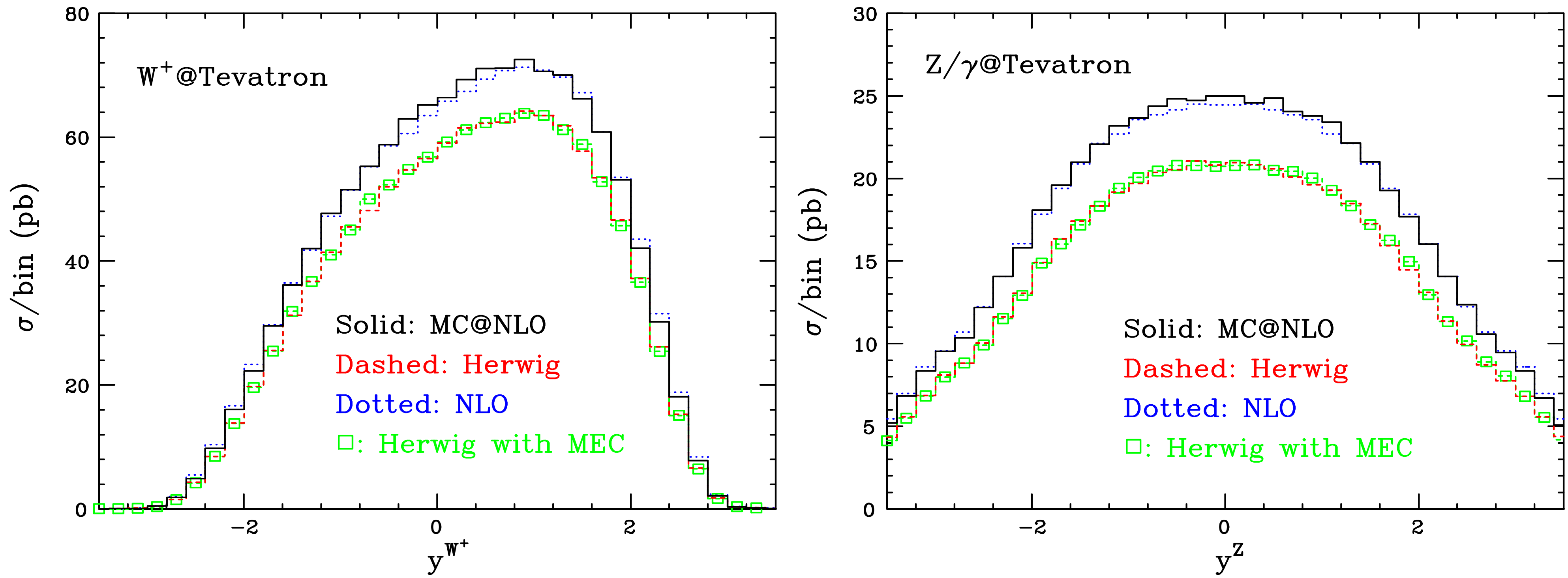
Is the agreement with the resummed result accidental?



The same happens with Higgs. The result of Bozzi, Catani, de Florian, Grazzini has a matching condition similar to MC@NLO, in that it conserves the total rate

- The agreement with the analytically-resummed result improves when the logarithmic accuracy of the latter is increased $\longrightarrow$ Herwig has more logs than you expect
- We can now apply any cuts we like (decay products, recoiling system) – a fully realistic jet-veto analysis is doable

MC@NLO and luminosity monitors



There is a good agreement between MC@NLO and NLO. NNLO contributions could perhaps be included by following the procedure advocated by Anastasiou, Dixon, Melnikov, Petriello, of multiplying by $\mathrm{K}^{(2)} = \sigma_{\mathrm{NNLO}}/\sigma_{\mathrm{NLO}}$

- However, $|\mathrm{MC@NLO} - \mathrm{NLO}| = \mathcal{O}(1-2\%)$ – may change with larger statistics
- A careful analysis, including realistic experimental cuts, is therefore necessary to decide whether Z and W production can be used as parton luminosity monitors in an analisys aimed at the 1% precision

Conclusions

NLOwPS's are theoretically well defined, and have reached the implementation stage. For them to become standard analysis tools *exp's feedback is essential*. NLOwPS's improve NLO computations and parton shower simulations in several respects

- MC@NLO is numerically more stable than NLO computations
- Realistic final states, including hadronization, are part of NLO predictions
- NLOwPS's are the only way in which K-factors can be embedded into MC's
- Hard radiation is incorporated in MC's, without the kinematical distortions of MEC

The presence of negative-weight events ($\sim 10\%$–20% in MC@NLO) is an unusual feature in MC's, which is however harmless. The major theoretical challenges for the future (and possible goals for the workshop):

- ♦ Increase the logarithmic accuracy of the showers
- ♦ Eliminate the negative weights (almost done!)