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# QCD at NLO: Monte Carlo developments

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# Higher orders versus MC's

| | *Good* | *Bad* | *Users* |
|---|---|---|---|
| HO | Hard emissions<br>Total rates | Soft&coll emissions<br>Hadronization<br>No events | Theorists |
| MC | Soft&coll emissions<br>Hadronization<br>Outputs events | Hard emissions<br>Total rates | Experimentalists |

In other words: $\mathrm{HO} \bigcap \mathrm{MC} = \emptyset$

A formalism incorporating HO *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 HO 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 (kind of new in HEP!)
- 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 HO computations is extremely naive, and strictly speaking can be applied only at very large $p_T$'s

# A less ambitious goal

The problem is much simplified if one selects only those Feynman diagrams contributing to HO, which correspond to the emissions of real particles

The improved MC is capable of simulating the emission of $n_E$ extra hard partons

Implicit is the notion of Born $\equiv$ LO level, the process(es) with the smallest number $n_B$ of final-state partons which contributes to a given reaction (usually $n_B = 2$)

This procedure is called Matrix Element Correction

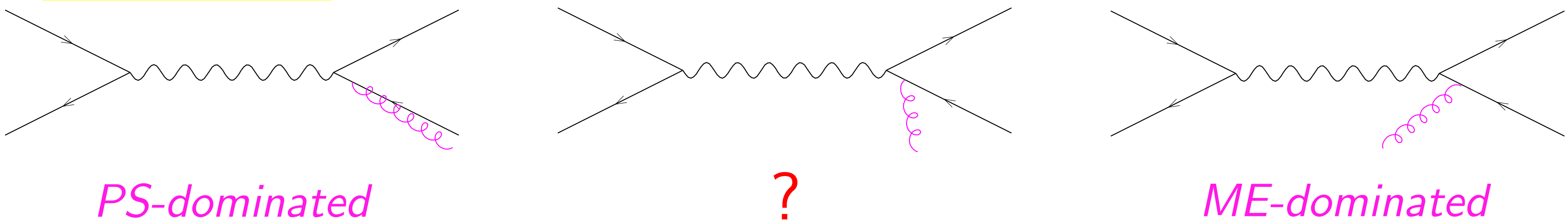
The strategy: generate the hard subprocesses with a standalone package (`AcerMC`, `ALPGEN`, `AMEGIC++`, `CompHEP`, `Grace`, `MadEvent`), and use the resulting kinematics as initital conditions for your favourite parton shower MC (`HERWIG`, `PYTHIA`)

- *Practical problems*: efficient ME generation for $(n_E + n_B)$-parton final states, efficient phase-space sampling
- *Principle problem*: real ME's diverge in the soft/collinear regions, and a cut $\delta_{sep}$ *must* be introduced at the parton level to avoid divergences $\Longrightarrow$ physical observables will depend on the unphysical $\delta_{sep}$ cutoff (a 20–30% effect at best)

# Getting rid of $\delta_{sep}$ dependence

In the context of $e^+e^-$ physics, Catani, Krauss, Kuhn & Webber show that the problem cannot be solved at fixed $n_B$. Extended to colour dipoles by Lönnblad; extended to hadronic collisions by Krauss

- **The problem:** $\delta_{sep}$ dependence $\Leftrightarrow$ double counting



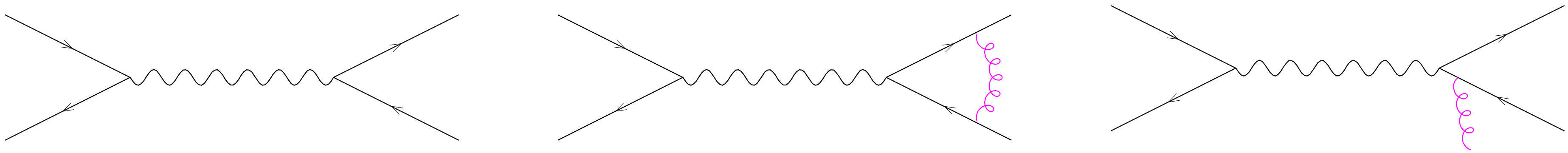

- **The solution:** separate the PS- and ME-dominated regions in an arbitrary manner; to compensate for the arbitrariness, the shower must be modified accordingly

- **The aim:** compute the observable at $\mathcal{O}(\alpha_S^{n-2})$, for any $n$, and resum to NLL accuracy (downstairs) where needed. By-product: the $\delta_{sep}$ dependence is reduced

$$\sigma_n \sim \alpha_S^{n-2} \sum_k a_k \alpha_S^k \log^{2k} \delta_{sep} \quad \longrightarrow \quad \alpha_S^{n-2} \left( \delta_{sep}^a + \sum_k b_k \alpha_S^k \log^{2k-2} \delta_{sep} \right)$$

# Adding virtual corrections: NLOwPS

The problem: virtual corrections pose additional difficulties



*Born* *Virtual* *Real*

The solution is unlikely to be unique, so 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 $\alpha_S$.
  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

NLO$^{n_E}$wPS with $n_E \neq 1$ is unfeasible with our present understanding

# NLOwPS versus MEC

■ Why is the definition of NLOwPS's much more difficult than MEC?

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

IR singularities are avoided in MEC by cutting them off with $\delta_{sep}$. This must be so, since only loop diagrams can cut off the divergences of real matrix elements

NLOwPS's are better than MEC since:

+ There is no $\delta_{sep}$ dependence

+ The computation of total rates is meaningful and reliable

NLOwPS's are worse than MEC since:

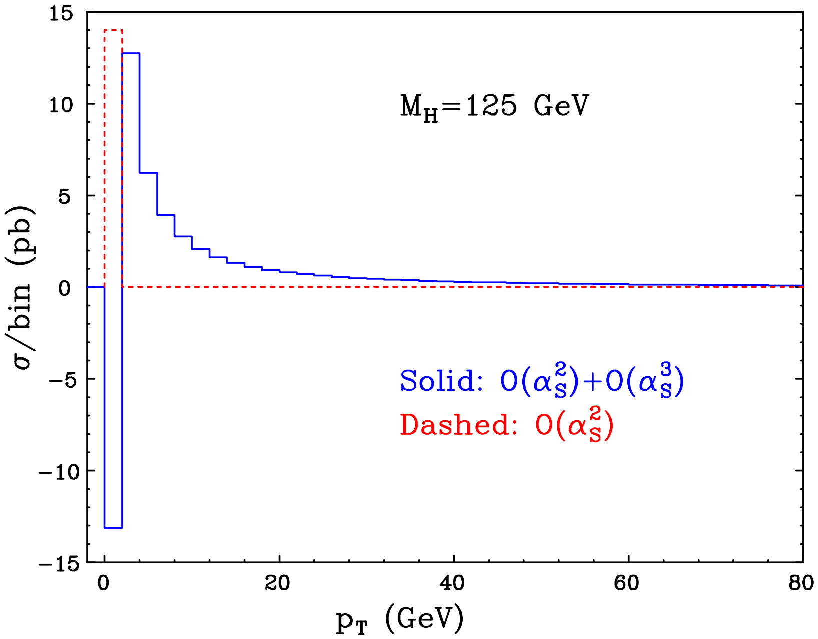
− The number of hard legs is smaller

− There are negative weights

A realistic goal: CKKW in NLOwPS's (i.e. multi-leg, NLO generators)

# 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$/\gamma$

- $\Phi$-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

- grcNLO (Kurihara *et al* – GRACE)
  Based on NLO hybrid slicing method, computes ME's numerically
  Double counts, if the parton shower is not built *ad hoc*
  Process implemented: $H_1 H_2 \longrightarrow$ Z

A proposal by Collins aims at including NLL effects in showers, but lacks gluon emission so far. $\Phi$-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)

# Fixed-order versus MC

## NLO cross section (based on subtraction)

$$\left(\frac{d\sigma}{dO}\right)_{subt} = \sum_{ab}\int dx_1\, dx_2\, d\phi_3\, f_a(x_1) f_b(x_2)$$
$$\Big[\delta(O - O(2\to 3))\mathcal{M}_{ab}^{(r)}(x_1, x_2, \phi_3) +$$
$$\delta(O - O(2\to 2))\Big(\mathcal{M}_{ab}^{(b,v,c)}(x_1, x_2, \phi_2) - \mathcal{M}_{ab}^{(c.t.)}(x_1, x_2, \phi_3)\Big)\Big]$$

## MC

$$\mathcal{F}_{\mathrm{MC}} = \sum_{ab}\int dx_1\, dx_2\, d\phi_2\, f_a(x_1) f_b(x_2)\, \mathcal{F}_{\mathrm{MC}}^{(2\to 2)}\mathcal{M}_{ab}^{(b)}(x_1, x_2, \phi_2)$$

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- Matrix elements $\longrightarrow$ normalization, hard kinematic configurations
- $\delta$-functions, $\mathcal{F}_{\mathrm{MC}}^{(2\to 2)} \equiv$ showers $\longrightarrow$ kinematic “evolution”

$$\Rightarrow \Big(\delta(O - O(2\to 2)), \delta(O - O(2\to 3))\Big) \longrightarrow \Big(\mathcal{F}_{\mathrm{MC}}^{(2\to 2)}, \mathcal{F}_{\mathrm{MC}}^{(2\to 3)}\Big) \ ?$$

# MC@NLO is based on a modified subtraction

The naive prescription doesn't work: MC evolution results in spurious NLO terms
We eliminate them by hand

- **MC@NLO**

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

$$
\boxed{\mathcal{M}_{\mathcal{F}(ab)}^{(\text{MC})} = \mathcal{F}_{\text{MC}}^{(2\to2)} \mathcal{M}_{ab}^{(b)} + \mathcal{O}(\alpha_S^2 \alpha_S^b)}
$$

There are *two* MC-induced contributions: they eliminate the spurious NLO terms due to the branching of a final-state parton, and to the non-branching probability

# Peculiarities of MC@NLO

Let's look at the weight functions

$$w_{\mathbb{H}}(\phi_3) = \mathcal{M}_{ab}^{(r)}(x_1, x_2, \phi_3) - \mathcal{M}_{ab}^{(\mathrm{MC})}(x_1, x_2, \phi_3)$$

$$w_{\mathbb{S}}(\phi_3) = \mathcal{M}_{ab}^{(b,v,c)}(x_1, x_2, \phi_2) - \mathcal{M}_{ab}^{(c.t.)}(x_1, x_2, \phi_3) + \mathcal{M}_{ab}^{(\mathrm{MC})}(x_1, x_2, \phi_3)$$

which are finite (i.e. don't diverge) for any $\phi_3$

**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

# 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

Negative weights don't mean negative cross sections. They arise from a different mechanism wrt those at the NLO, and their number is fairly limited

# MC@NLO 2.31 [hep-ph/0402116]

| IPROC | Process |
|---|---|
| –1350–IL | $H_1H_2 \to (Z/\gamma^* \to) l_{\rm IL}\bar{l}_{\rm IL} + X$ |
| –1360–IL | $H_1H_2 \to (Z \to) l_{\rm IL}\bar{l}_{\rm IL} + X$ |
| –1370–IL | $H_1H_2 \to (\gamma^* \to) l_{\rm IL}\bar{l}_{\rm IL} + X$ |
| –1460–IL | $H_1H_2 \to (W^+ \to) l^+_{\rm IL}\nu_{\rm IL} + X$ |
| –1470–IL | $H_1H_2 \to (W^- \to) l^-_{\rm IL}\bar{\nu}_{\rm IL} + X$ |
| –1396 | $H_1H_2 \to \gamma^*(\to \sum_i f_i\bar{f}_i) + X$ |
| –1397 | $H_1H_2 \to Z^0 + X$ |
| –1497 | $H_1H_2 \to W^+ + X$ |
| –1498 | $H_1H_2 \to W^- + X$ |
| –1600–ID | $H_1H_2 \to H^0 + X$ |
| –1705 | $H_1H_2 \to b\bar{b} + X$ |
| –1706 | $H_1H_2 \to t\bar{t} + X$ |
| –2850 | $H_1H_2 \to W^+W^- + X$ |
| –2860 | $H_1H_2 \to Z^0Z^0 + X$ |
| –2870 | $H_1H_2 \to W^+Z^0 + X$ |
| –2880 | $H_1H_2 \to W^-Z^0 + X$ |

- Works identically to HERWIG: the very same analysis routines can be used
- Reads shower initial conditions from an event file (as in ME corrections)
- Exploits Les Houches accord for process information and common blocks
- Features a self contained library of PDFs with old and new sets alike
- LHAPDF will also be implemented

# NLOwPS: $\Phi$-veto

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

$$\int_{\phi_0} d\phi_3 \left( \mathcal{M}_{ab}^{(b,v,c)} + \mathcal{M}_{ab}^{(r)} \right) = 0$$

Another (freely defined) phase-space region $\phi_H \subset \phi_0$ is populated by hard-emission events (Pötter, Schörner, Dobbs)

$$\begin{aligned}
\mathcal{F}_{\Phi_{\text{veto}}} \quad = \quad & \sum_{ab} \int dx_1\, dx_2\, d\phi_3\, f_a(x_1) f_b(x_2) \\
& \Big[ \mathcal{F}_{\text{MC}}^{(2\to3)} \mathcal{M}_{ab}^{(r)}(x_1, x_2, \phi_3)\, \Theta(\phi_3 \in \phi_H) + \\
& \mathcal{F}_{\text{MC}}^{(2\to2)} \mathcal{M}_{ab}^{(b,v,c)}(x_1, x_2, \phi_2)\, \Theta\big(\phi_3 \in \overline{\phi_0} \cap \overline{\phi_H}\big) + \Big]
\end{aligned}$$

$+$ *Only positive weights*

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

$-$ *Double counting for $\phi_3 \in \overline{\phi_H}$, and discontinuity at $\partial\phi_H$ imply dependence upon $\phi_H$, which is hidden by integration over Bjorken $x$'s*

$-$ *Strictly speaking, the (perturbative) result is non-perturbative ($\phi_0 \sim \exp(-1/\alpha_S)$)*

# NLOwPS: grcNLO

Partition the phase space as in standard slicing (i.e., define a non-soft, non collinear region $\phi_{NSC}$), and subtract there the real counterterm:

$$\begin{aligned}\mathcal{F}_{\text{grcNLO}} &= \sum_{ab}\int dx_1\, dx_2\, d\phi_3\, f_a(x_1) f_b(x_2) \\ &\Big[\mathcal{F}_{\text{MC}}^{(2\to 3)}\left(\mathcal{M}_{ab}^{(r)}(x_1,x_2,\phi_3) - \mathcal{M}_{ab}^{(c.t.)}(x_1,x_2,\phi_3)\right)\Theta(\phi_3\in\phi_{NSC}) + \\ &\mathcal{F}_{\text{MC}}^{(2\to 2)}\mathcal{M}_{ab}^{(b,v,c)}(x_1,x_2,\phi_2)\Big]\end{aligned}$$

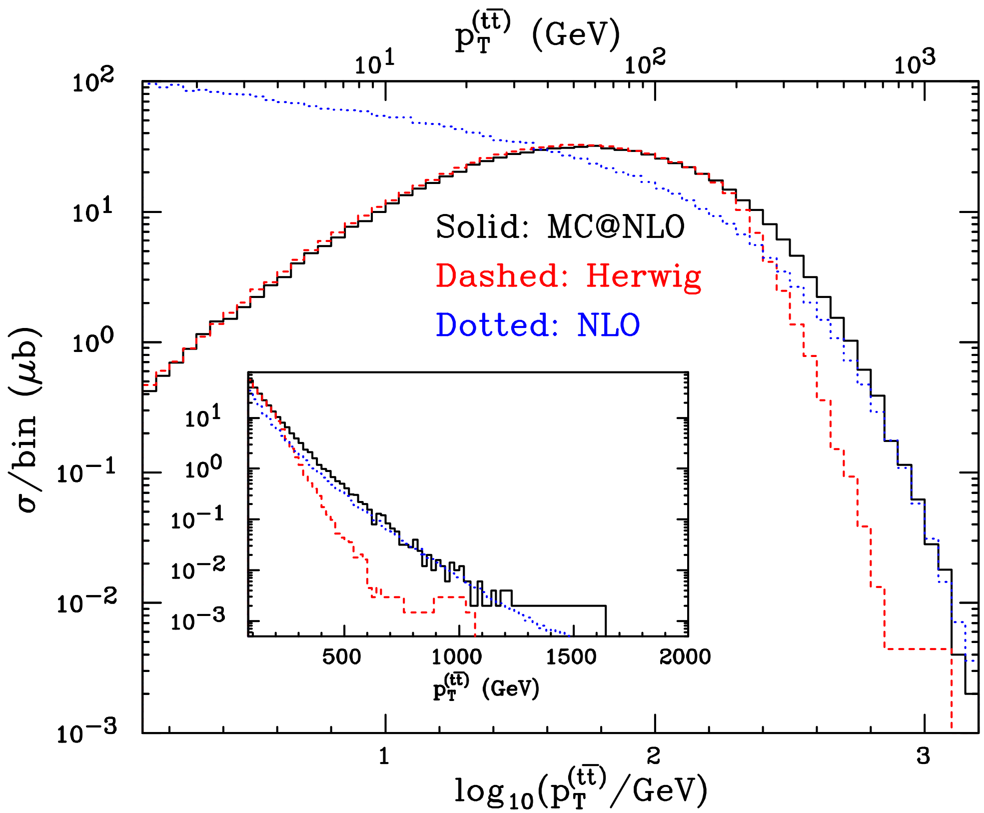
This formally coincides with MC@NLO, provided that $\phi_{NSC}$ *is* the full phase space, and

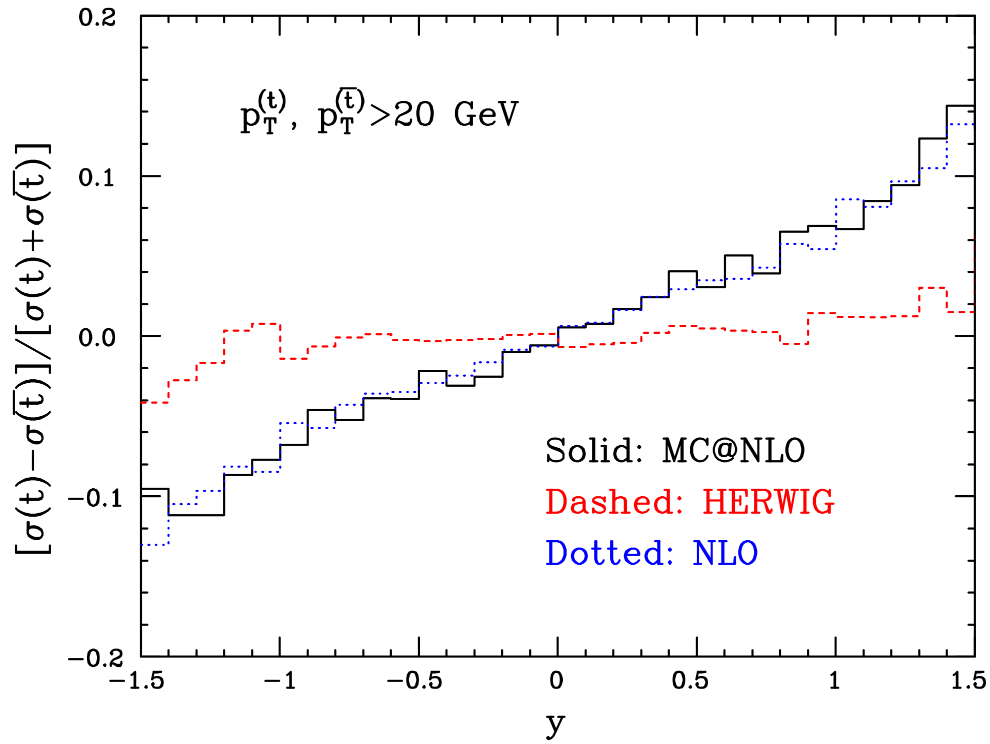
$$\mathcal{M}_{ab}^{(\text{MC})} \equiv \mathcal{M}_{ab}^{(c.t.)}$$

This condition cannot be imposed: it must result from the MC implementation

+ *All matrix elements generated numerically*
− *Double counting if $\mathcal{M}_{ab}^{(MC)}$ is not built* ad hoc
− *Condition on $\mathcal{M}_{ab}^{(MC)}$ implies the construction of a new MC*

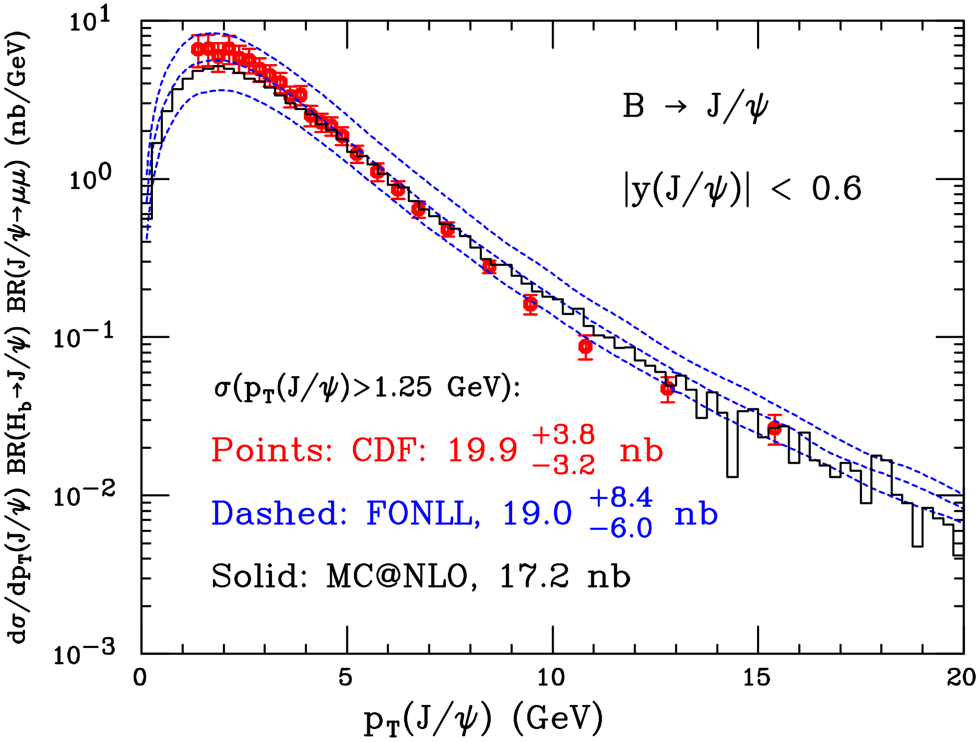
# What to expect from an NLOwPS (here MC@NLO)

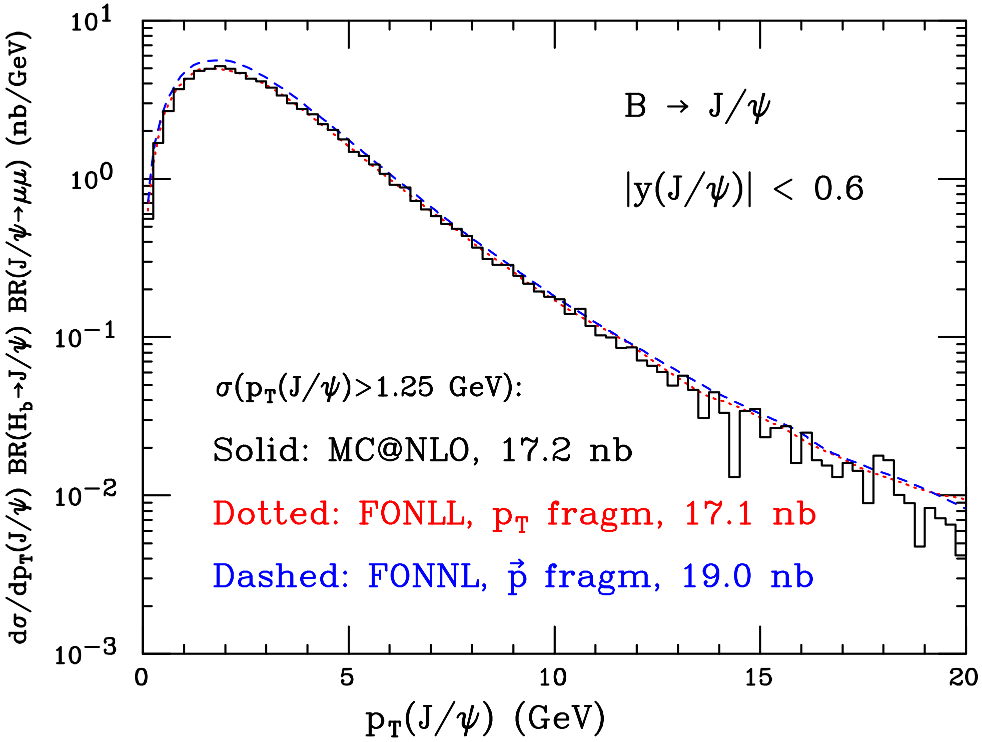



- MC@NLO rate = NLO rate $\Longrightarrow$ K-factors are included consistently
- MC@NLO- and MC-predicted shapes are identical where MC does a good job
- $\mathcal{S}$+0 jet and $\mathcal{S}$+1 jet treated exactly, $\mathcal{S}+n$ jets $(n > 1)$ better than in MC's
- No dependence on $\delta_{sep}$ $\Longrightarrow$ tuning is the same as in ordinary MC's
- Some negative-weight events, to be subtracted (rather than added) from histograms

# Single-inclusive $b$ at the Tevatron

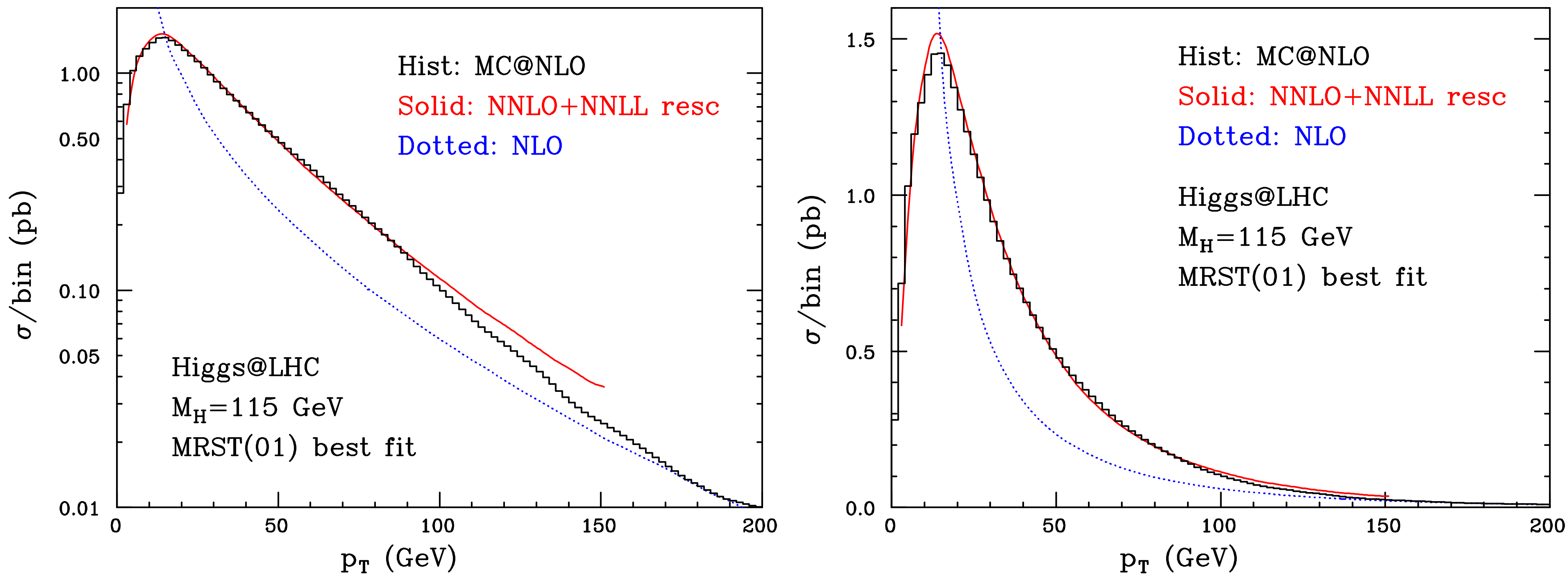



No significant discrepancy with data

- No PTMIN dependence in MC@NLO $\Longrightarrow$ solid predictions down to $p_T = 0$, no "perturbative-parameter tuning" (more work on $b$ hadronization parameters needed)
- 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
- Beware: vastly different from Pythia!

# Conclusions

There has been substantial theoretical progress in MC's in the past three years or so. The timing is just right, since it's the Tevatron and the LHC that demand the construction of improved MC tools

MEC for multileg processes are firmly established

- Expect CKKW to become part of HERWIG, PYTHIA, and SHERPA releases
- Reliable estimates for many backgrounds to new physics

NLOwPS's improve NLO computations and MC 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 any kinematical distortion

NLOwPS/MEC work just like ordinary MC's, and must be seen as upgrades of the latter. So the answer to the question: when do I have to use them? is: always