

Stefano Frixione

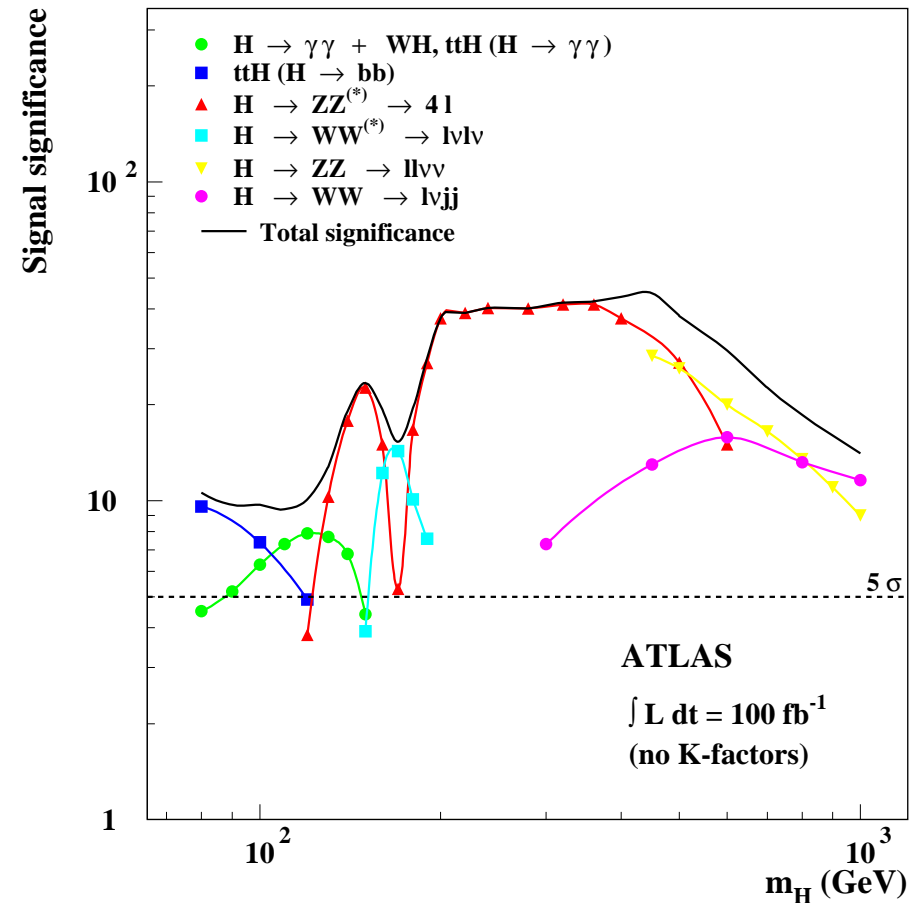
Generatori di eventi:  
progressi in vista di LHC

Napoli, 13/10/2004

# Monte Carlos and hadronic physics

Whether Monte Carlos are discovery tools is a debatable issue

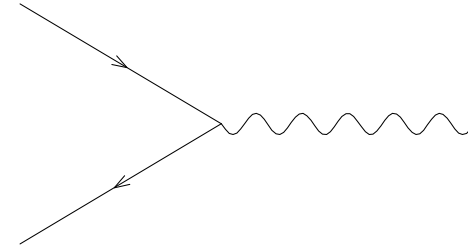
- A striking feature, such as a narrow mass peak, would render the use of MC's fairly marginal to claim a discovery
- A counting experiment has to rely on firm control of standard model predictions. Rates *may* be normalized to data, shapes have to be predicted as accurately as possible – e.g. the (gone) large- $E_T$  jet excess @ Tevatron



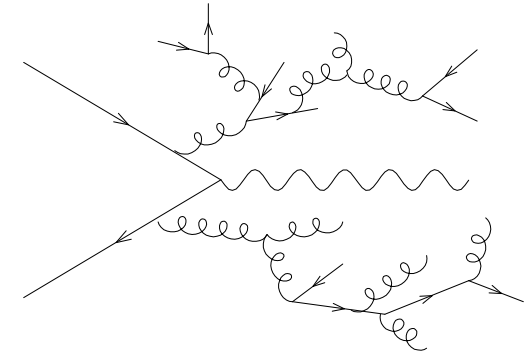
Independently of the scenario we'll face, MC's will play a central role in our understanding of LHC physics. So the relevant question to ask is whether standard MC's are up to the task

# Physics processes with standard MC's

1) Compute the LO cross section in perturbation theory



2) Let the shower emit as many gluons and quarks as possible



## Advantages

- The analytical computations are trivial
- Very flexible
- Resum (at least) leading logarithmic contributions

## Drawbacks

- The high- $p_T$  and multijet configurations are not properly described
- The total rate is computed to LO accuracy

These problems stem from the fact that the MC's perform the showers assuming that all emissions are collinear

# So what?

Experimenters don't have the radical-chic attitude of theorists. They take a code (full of bugs), make it run, multiply the result by the  $K$  factor (whatever this means), perhaps add a  $k_T$ -kick (no one definitely knows what *this* means), rescale, reweight, ...

and it works!

At least, it worked up to now. What are the reasons to suspect that things may change?

- The one sure thing about LHC: the central role of processes with many well separated jets and/or large  $K$  factors. These are precisely the features that standard MC's cannot predict well
- A lesson from the past: to achieve their flagship accuracies, LEP experiments have accurately tuned their MC's (and thus thoroughly tested them), and used them in conjunction with other kind of codes (typically, fixed-order computations). There is no comparable expertise in hadronic collider experiments

The bottom line: it's LHC physics that demands the MC's be improved.  
If MC's miss gross kinematic features, they cannot possibly describe data

# How to improve Monte Carlos?

We need to consider fixed-order computations\* in perturbation theory, since they:

- ◆ Correctly account for hard emissions
- ◆ Estimate reliably total rates
- ◆ Reduce the impact of unphysical mass scales, and allow one to accurately determine the unknowns of the theory, such as  $\alpha_s$  and PDFs

In other words, fixed-order computations perform well where MC's fail. The opposite is also true. The two approaches are thus complementary

To what extent can we combine the powerful features of perturbative computations and of Monte Carlo simulations in a single formalism?

\* I won't discuss perspectives for Underlying Events – lot of work done (modelling and tuning), but still sort of plug & pray for LHC. Needs deeper theoretical understanding

# Higher orders + MC's $\implies$ ?

How does a formalism with all the **Good** features look like?

We should take into account that:

- 1) MC's are the natural frameworks in which realistic hadronization models can be implemented (power corrections are important – see LEP)
- 2) MC's output events which mimic those occurring in Nature, and this renders the MC's suitable to theoretical and experimental analyses alike
- 3) MC's effectively perform the resummations of large classes of logarithmic terms

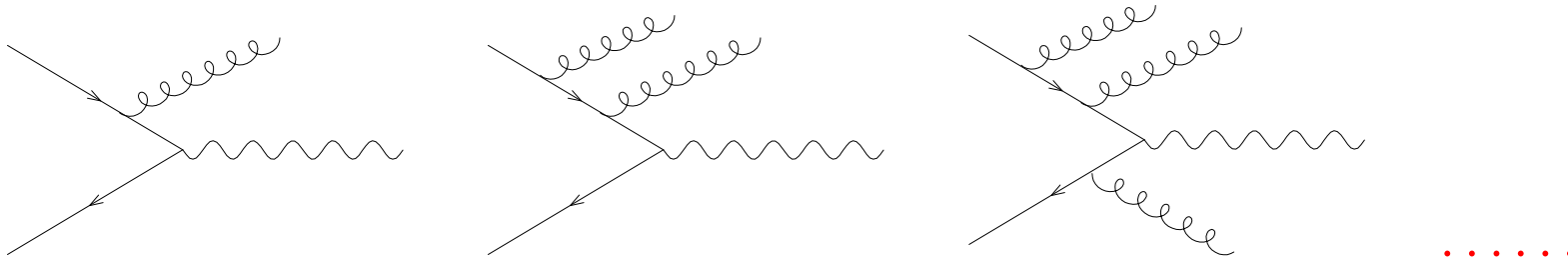
Items 1) and 2) imply that we should start with a MC, and embed in it as much information as possible on higher-order computations

Item 3) implies that, by doing so, resummed **and matched** results will automatically be recovered

How can we insert higher-order matrix elements into Monte Carlos?

# Matrix Element Corrections

Just compute (exactly) more **real emission** diagrams before starting the shower



## Problems

- Double counting (the shower can generate the same diagrams)
- The diagrams are divergent

## Solution

Cut the divergences off by means of an arbitrary parameter  $\delta_{sep}$

$\implies$  **physical** observables will depend on the **unphysical**  $\delta_{sep}$  cutoff

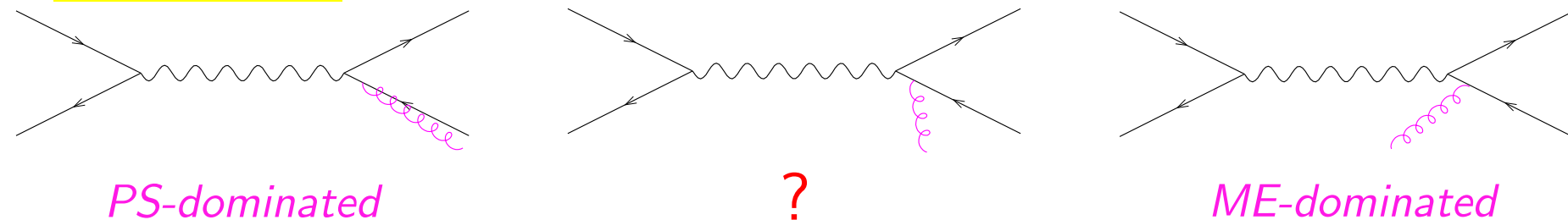
Hard subprocesses are typically generated with a standalone package (**AcerMC**, **ALPGEN**, **AMEGIC++**, **CompHEP**, **Grace**, **MadEvent**), which must be efficient in:

*a)* computing the matrix elements; *b)* sampling the phase space for unweighting

# 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 number of hard legs**. Extended to colour dipoles by [Lönnblad](#); extended to hadronic collisions by [Krauss](#); alternative (simpler) strategy by [Mangano](#)

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



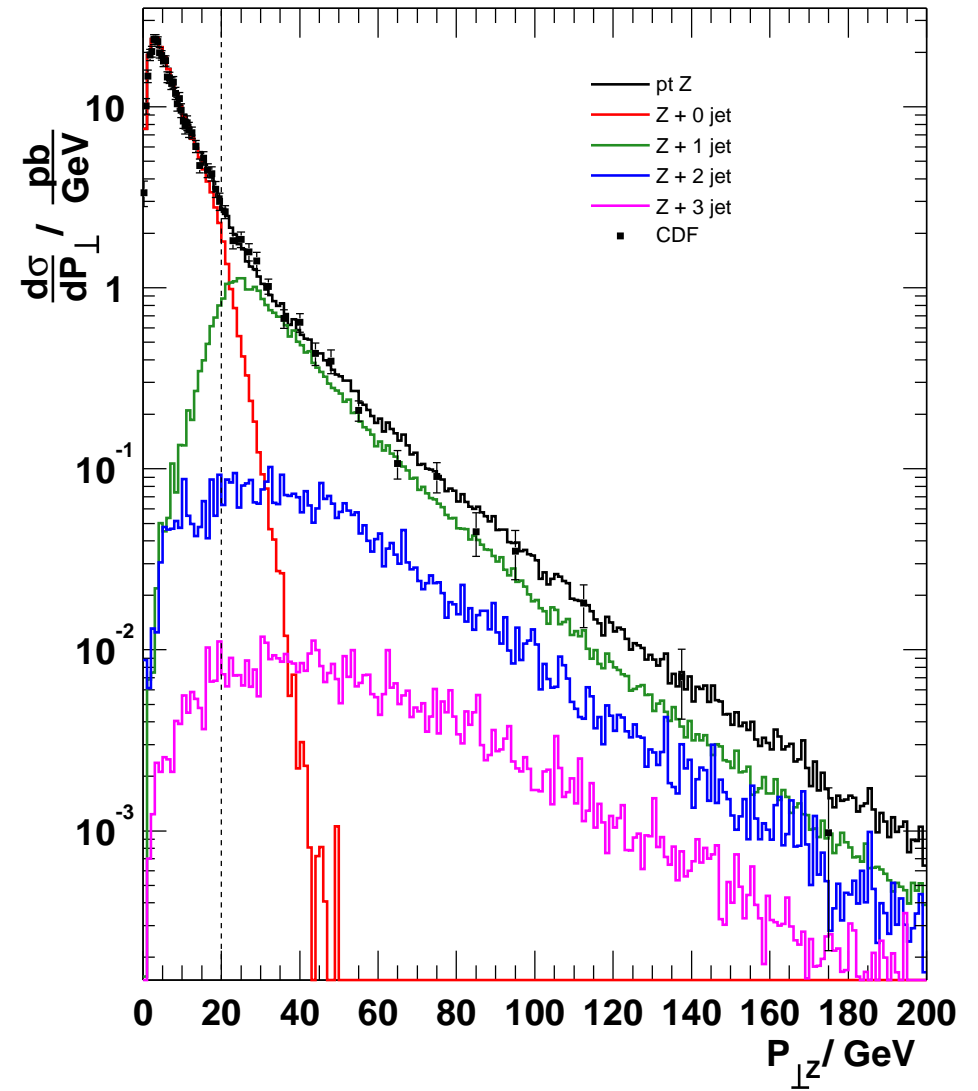
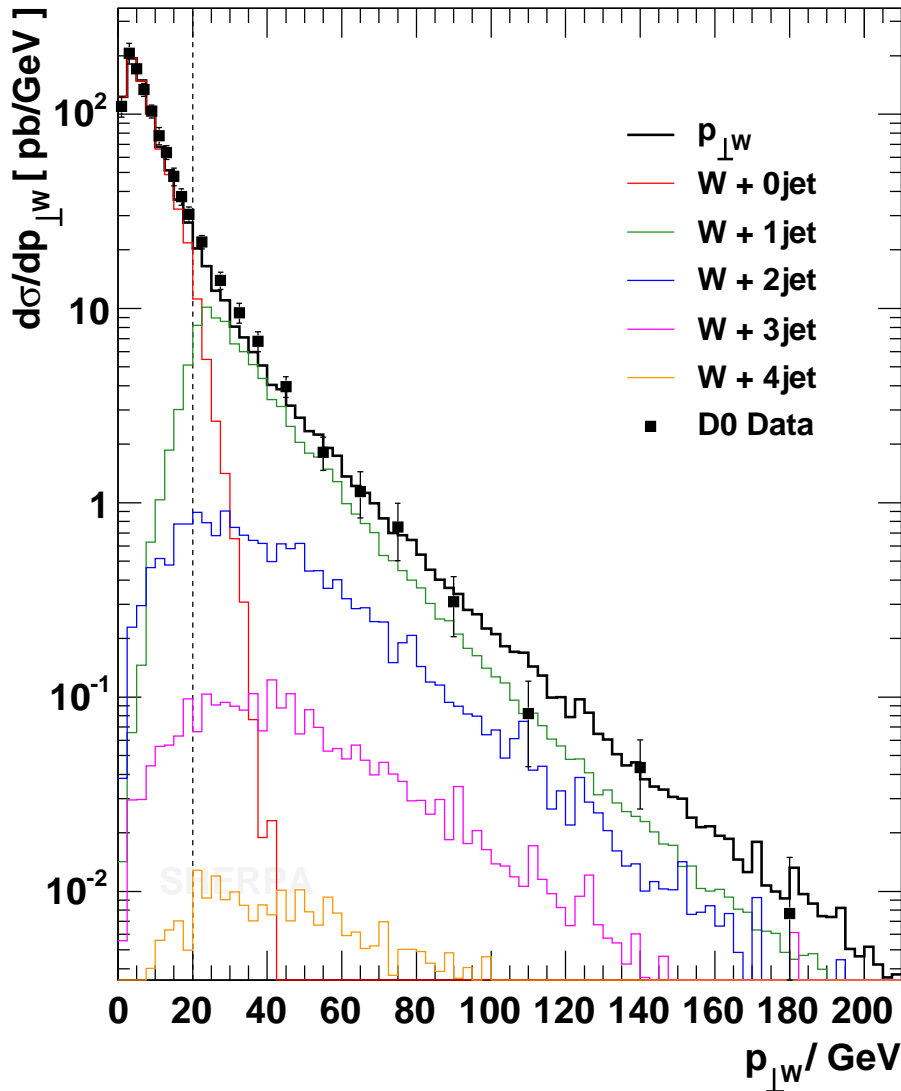
- **The solution:** separate the PS- and ME-dominated regions in an **arbitrary** manner; to compensate for the arbitrariness, the **shower and ME's must be modified** accordingly

- **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

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



# Using MEC

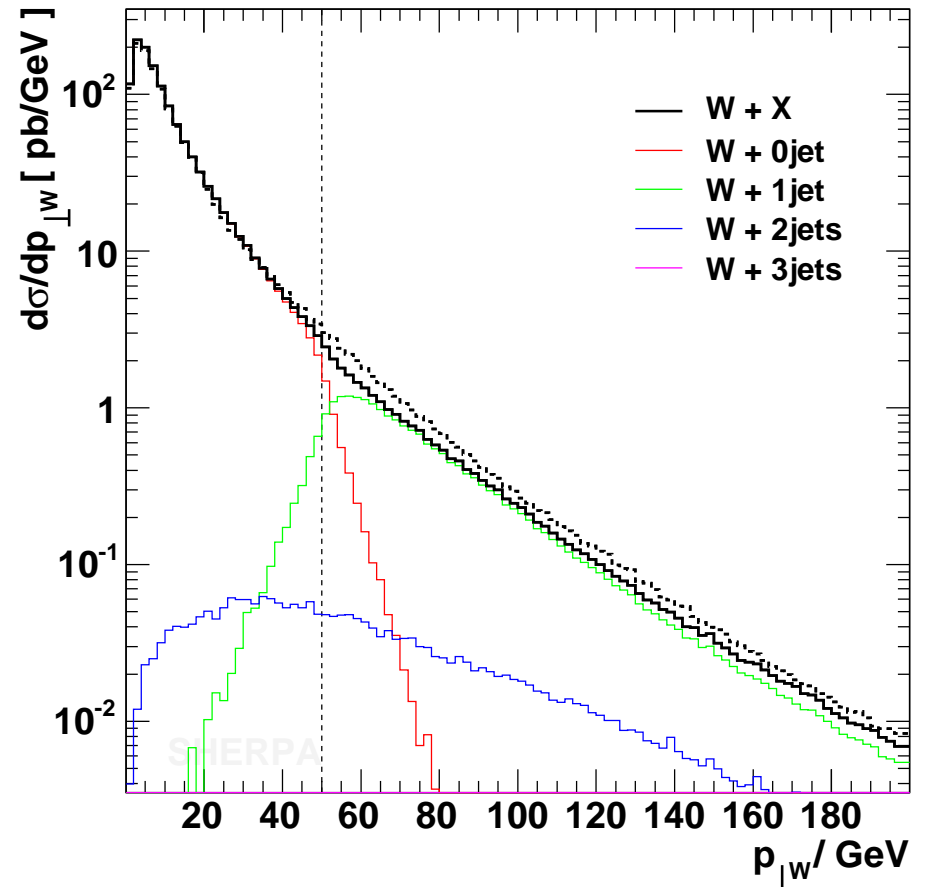
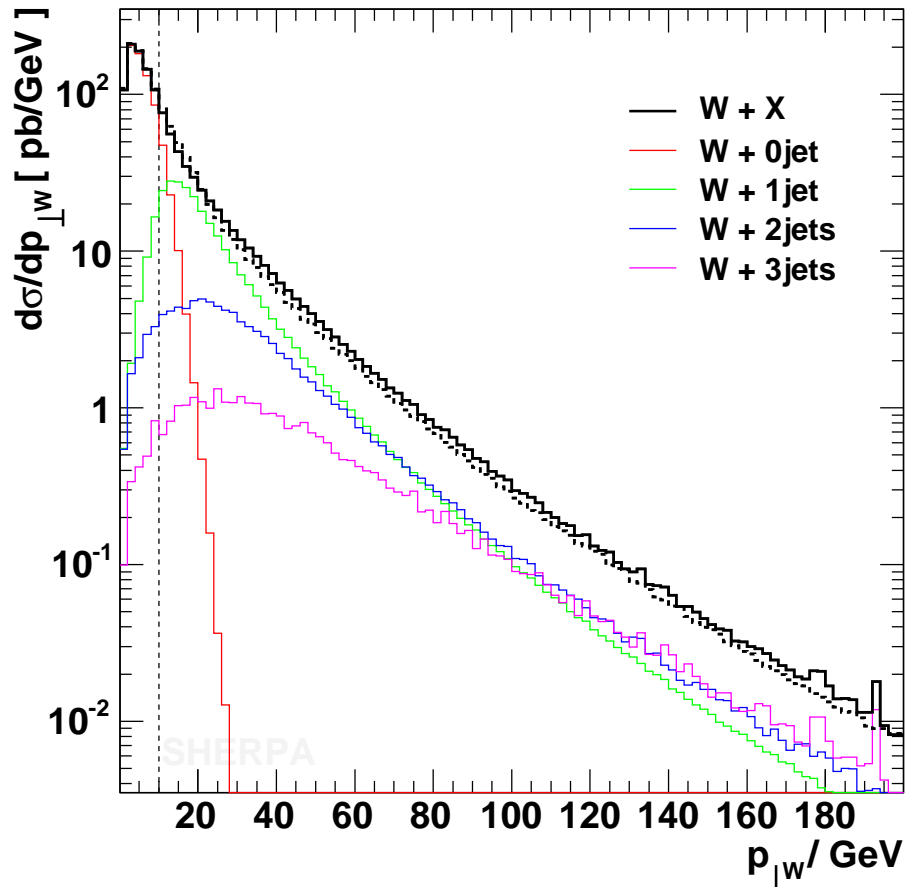


SHERPA (from hep-ph/0409122) – CKKW is built in

Different partonic subprocesses cooperate to give the physical result

■ How about the  $\delta_{sep}$  dependence?

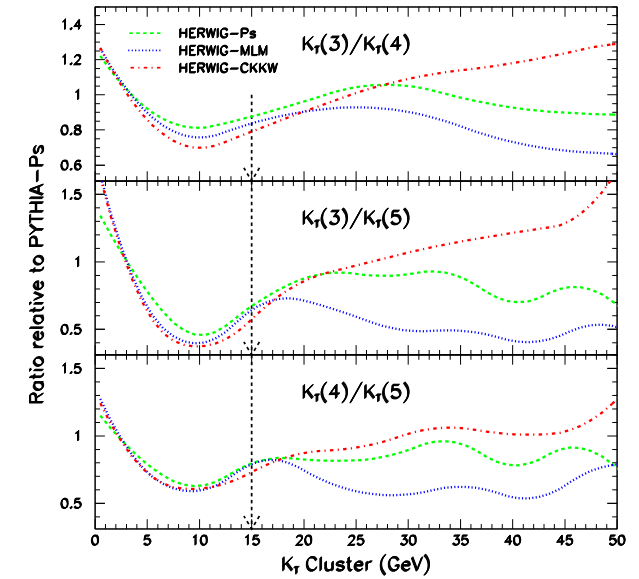
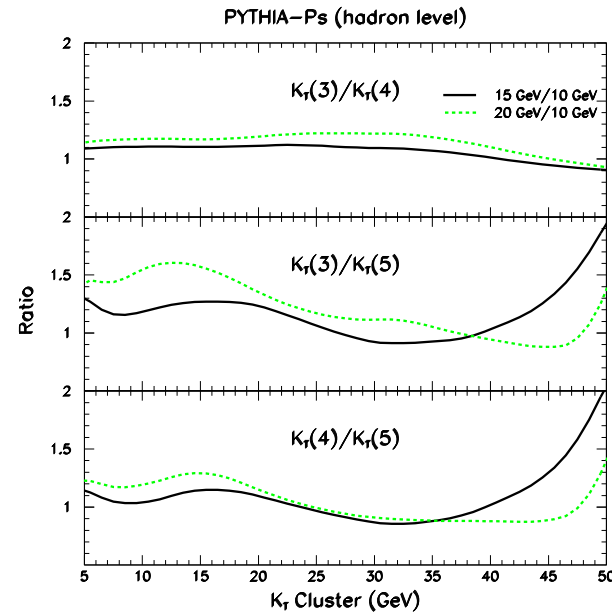
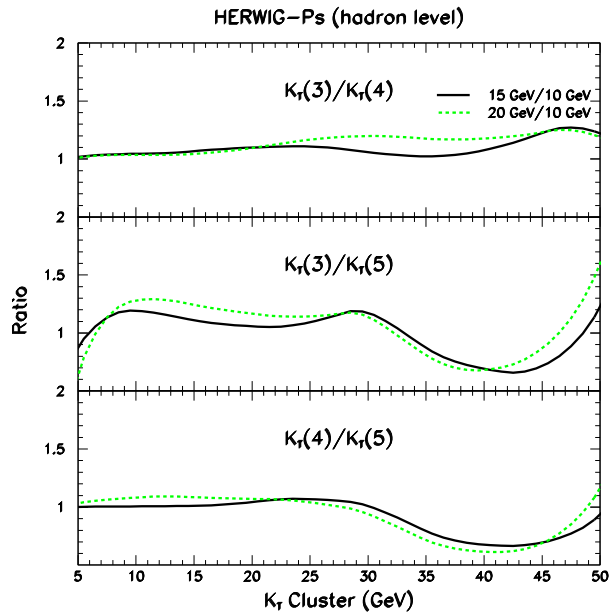
# $\delta_{sep}$ effects on observables I



SHERPA (from hep-ph/0409122)

In hadronic collisions,  $\delta_{sep}$  is dimensionful ( $Q_{cut}$ ). It is reassuring that, in spite of the large dependence on  $Q_{cut}$  of the individual partonic subprocesses, the physical result is decently stable. The residual dependence may be used to tune the MC to data

# $\delta_{sep}$ effects on observables II



## HERWIG and PYTHIA (Richardson & Mrenna, hep-ph/0312274)

The  $\delta_{sep}$  dependence appears here to be larger than for  $p_T^{(W)}$ ; furthermore, there are differences between implementations of different matching procedures in the same MC, and of the same matching procedure in different MC's

- Matching systematics must be carefully assessed for each observable studied, using at least two different MC's

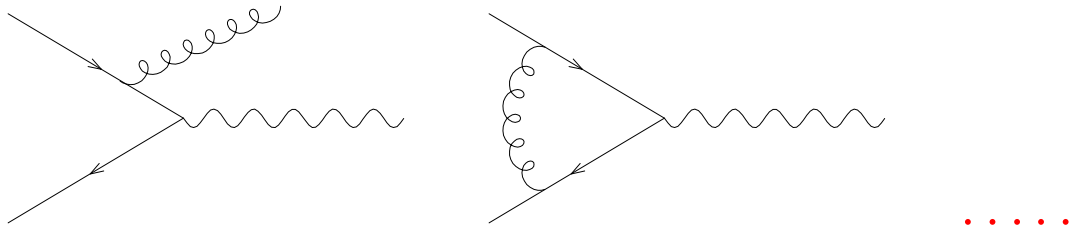
## A short summary on MEC

- ◆ MEC have come a long way since the mid-90's works of [Sjöstrand](#) and [Seymour](#)
- ◆ Old-fashioned MEC are basically impossible to apply to anything but processes whose radiation and colour patterns are simple
- ◆ New MEC are formally established in  $e^+e^-$  collisions; similar formal proofs are lacking in hadronic collisions, but implementations appear robust
- ◆ Although no principle problems have to be expected, it is mandatory to check that these techniques work with processes more involved than  $W + n$  jets (e.g. preliminary D0 2-jet studies – perhaps 2 is not a large number)
- ◆ The dependence upon the unphysical  $\delta_{sep}$  is a mixed blessing. The substantial amount of work done for  $W + n$  jets *may need* be done again for other processes. On the other hand, the residual  $\delta_{sep}$  dependence gives an extra lever arm for tuning on data

No sensible predictions for multi-jet observables can be obtained with standard MC's. MEC implementations in MC's must be used in physics simulations before the LHC starts – experimenters' feedback is essential to spark further improvements

# Adding virtual corrections: NLOwPS

Compute **all NLO diagrams** before starting the shower



## Problems

- Double counting (the shower can generate the same diagrams)
- The diagrams are divergent

## Solution (MC@NLO)

Remove the divergences locally by **adding and subtracting the MC result** that one would get after the first emission (**yes, this is sufficient!**)

Virtual diagrams cancel the divergences of the real diagrams, and therefore it is not necessary to introduce  $\delta_{sep}$ ; as a by-product, total rates are computed to NLO accuracy. No parameter tuning is involved in the procedure (there are no arbitrary parameters)

# NLOwPS versus MEC

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

The problem is a serious 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 (i.e., no merging systematics)
- + The computation of total rates is meaningful and reliable

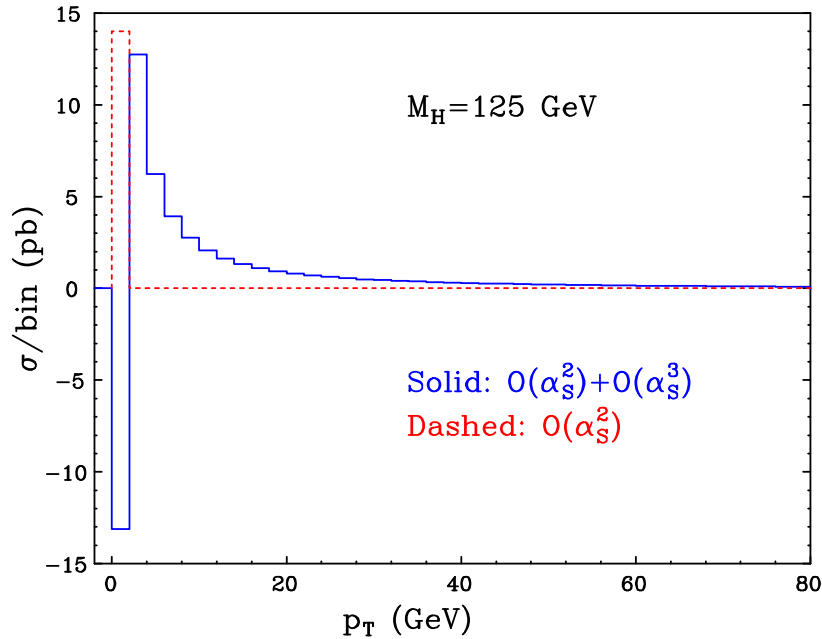
NLOwPS's are worse than MEC since:

- The number of hard legs is smaller
- There are negative weights (i.e., more running time required)

A realistic goal for the near future: multi-leg NLOwPS's

# What does NLO mean?

Consider Higgs production:



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

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

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

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

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; 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  $e^+ e^- \rightarrow 3$  jets (but without a realistic MC)



# NLO and MC computations

## ■ NLO cross section (based on subtraction)

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

## ■ MC

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

◆ Matrix elements  $\longrightarrow$  normalization, hard kinematic configurations

◆  $\delta$ -functions,  $\mathcal{F}_{MC}^{(2 \rightarrow 2)} \equiv$  showers  $\longrightarrow$  kinematic “evolution”

$$\implies \left( \delta(O - O(2 \rightarrow 2)), \delta(O - O(2 \rightarrow 3)) \right) \longrightarrow \left( \mathcal{F}_{MC}^{(2 \rightarrow 2)}, \mathcal{F}_{MC}^{(2 \rightarrow 3)} \right) ?$$

# MC@NLO is based on a modified subtraction

The naive prescription doesn't work: MC evolution results in spurious NLO terms

→ Eliminate the spurious NLO terms "by hand"

## ■ MC@NLO

$$\mathcal{F}_{\text{MC@NLO}} = \sum_{ab} \int dx_1 dx_2 d\phi_3 f_a(x_1) f_b(x_2) \left[ \mathcal{F}_{\text{MC}}^{(2 \rightarrow 3)} \left( \mathcal{M}_{ab}^{(r)}(x_1, x_2, \phi_3) - \mathcal{M}_{ab}^{(\text{MC})}(x_1, x_2, \phi_3) \right) + \mathcal{F}_{\text{MC}}^{(2 \rightarrow 2)} \left( \mathcal{M}_{ab}^{(b,v,c)}(x_1, x_2, \phi_2) - \mathcal{M}_{ab}^{(c.t.)}(x_1, x_2, \phi_3) + \mathcal{M}_{ab}^{(\text{MC})}(x_1, x_2, \phi_3) \right) \right]$$

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

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

# 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)

$$\begin{aligned} \mathcal{F}_{\Phi_{\text{veto}}} = & \sum_{ab} \int dx_1 dx_2 d\phi_3 f_a(x_1) f_b(x_2) \\ & \left[ \mathcal{F}_{\text{MC}}^{(2 \rightarrow 3)} \mathcal{M}_{ab}^{(r)}(x_1, x_2, \phi_3) \Theta(\phi_3 \in \phi_H) + \right. \\ & \left. \mathcal{F}_{\text{MC}}^{(2 \rightarrow 2)} \mathcal{M}_{ab}^{(b,v,c)}(x_1, x_2, \phi_2) \Theta(\phi_3 \in \overline{\phi_0} \cap \overline{\phi_H}) + \right] \end{aligned}$$

- + 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:

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

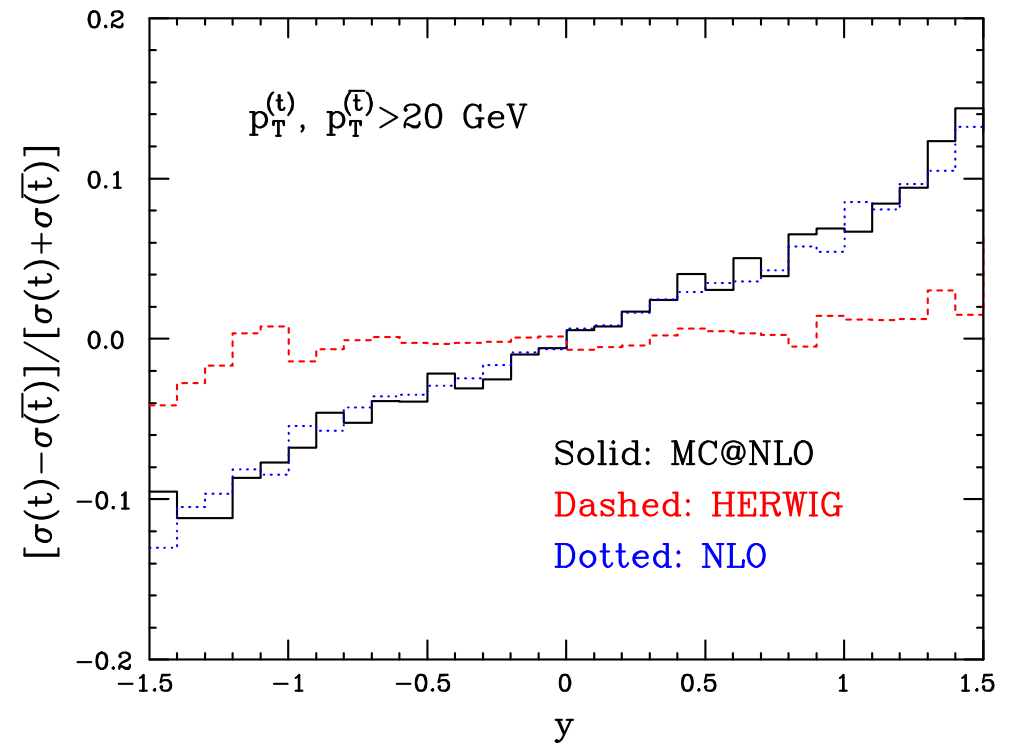
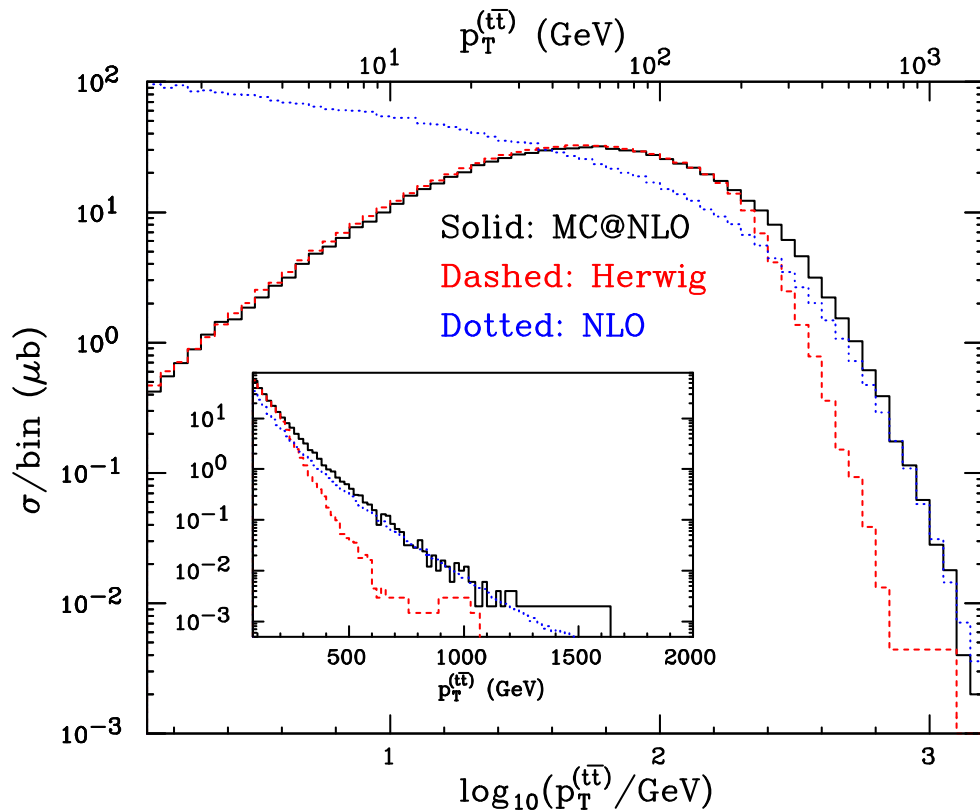
This formally coincides with MC@NLO, provided that  $\phi_{NSC}$  is the full phase space, and

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

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

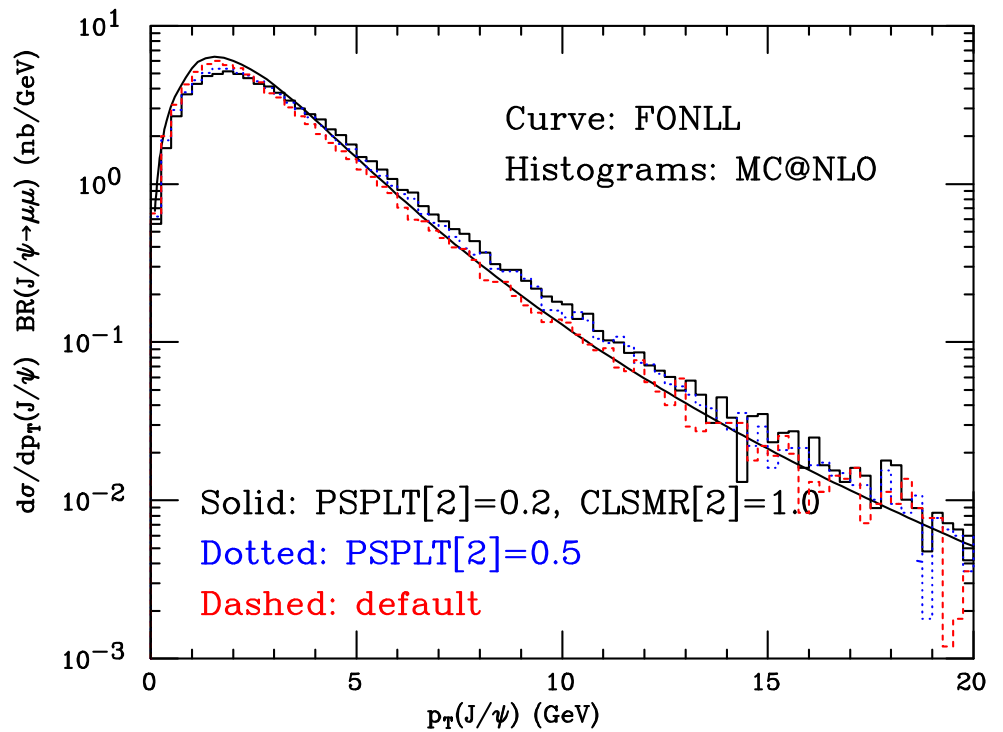
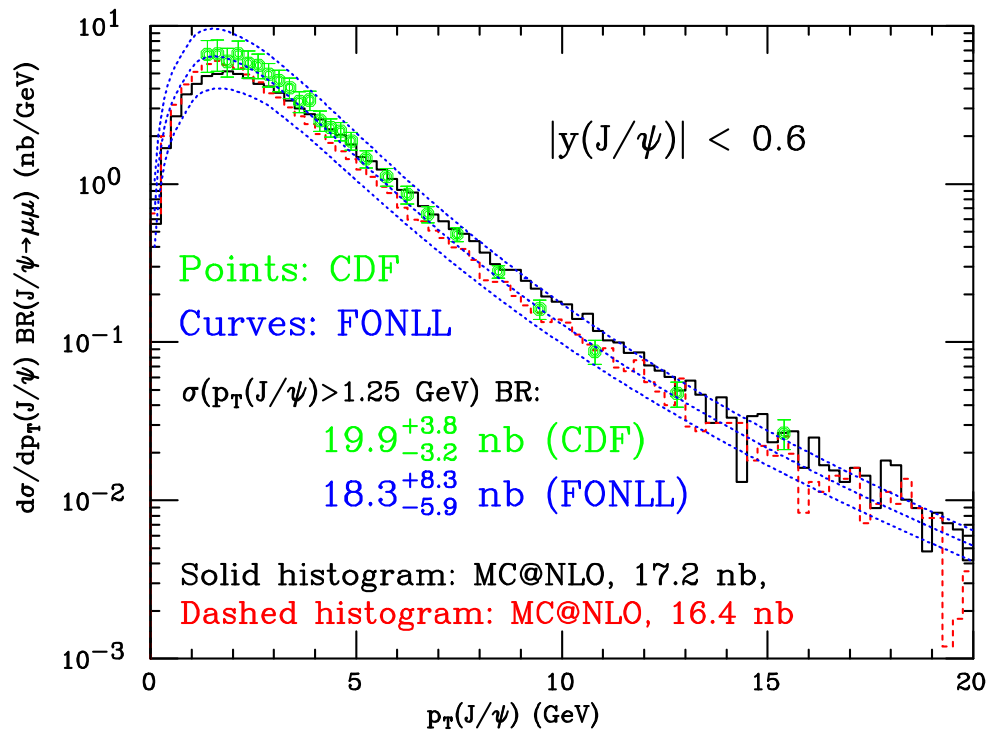
- + *All matrix elements generated numerically*
- *Double counting* if  $\mathcal{M}_{ab}^{(\text{MC})}$  is not built ad hoc
- *Condition on  $\mathcal{M}_{ab}^{(\text{MC})}$  implies the construction of a new MC*

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



- MC@NLO rate = NLO rate  $\implies$  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  $\delta_{sep}$   $\implies$  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

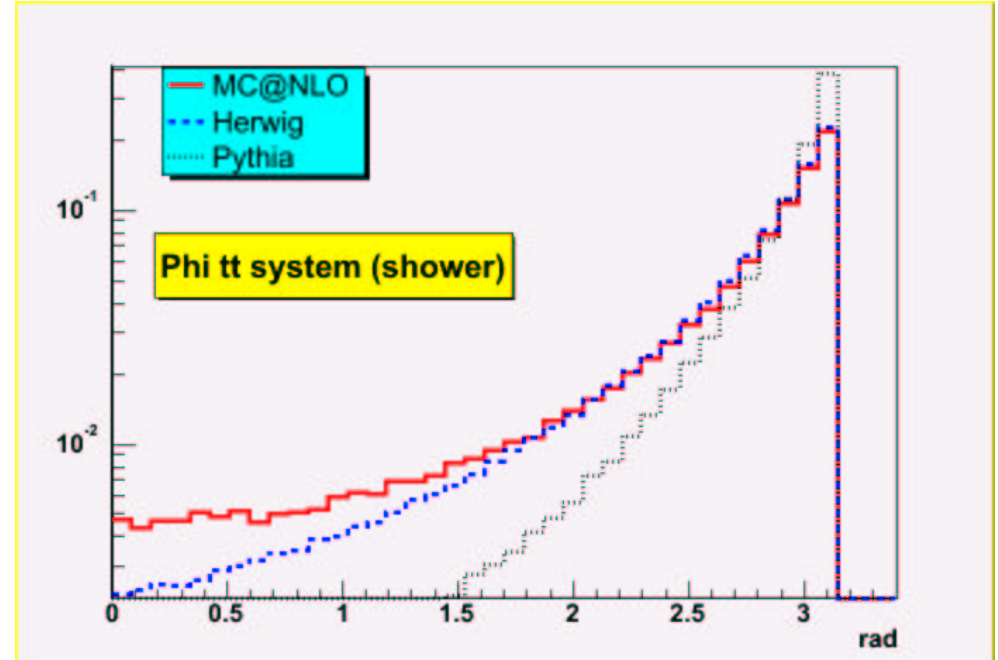
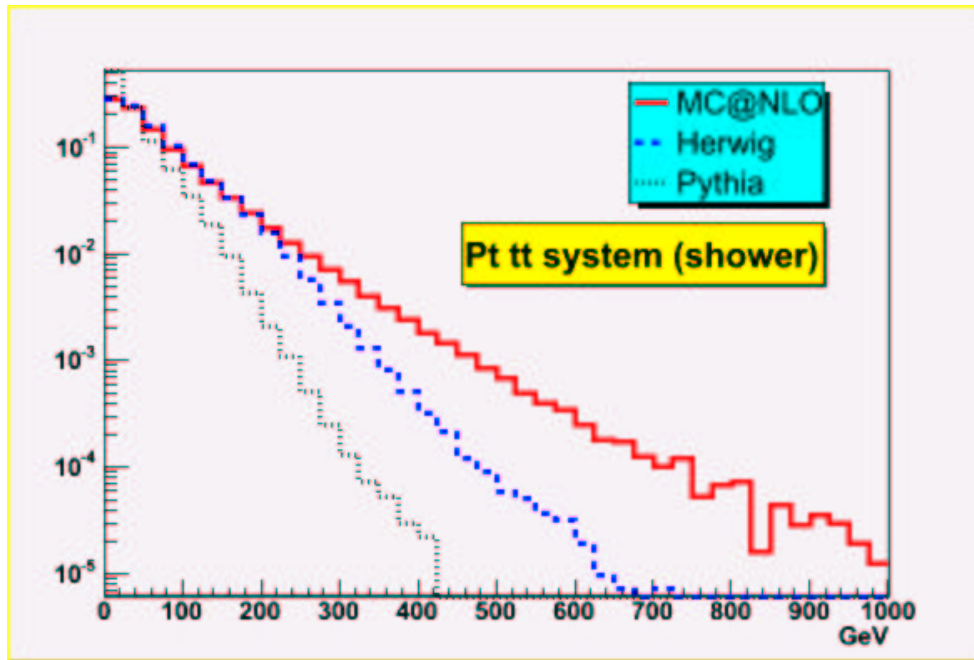


No significant discrepancy with data

- No PTMIN dependence in MC@NLO  $\implies$  solid predictions down to  $p_T = 0$
- Full agreement with NLL+NLO computation (FONLL, Cacciari&Nason)

$\longrightarrow$  Del Duca, Cacciari

# A case study: $t\bar{t}$ at LHC I

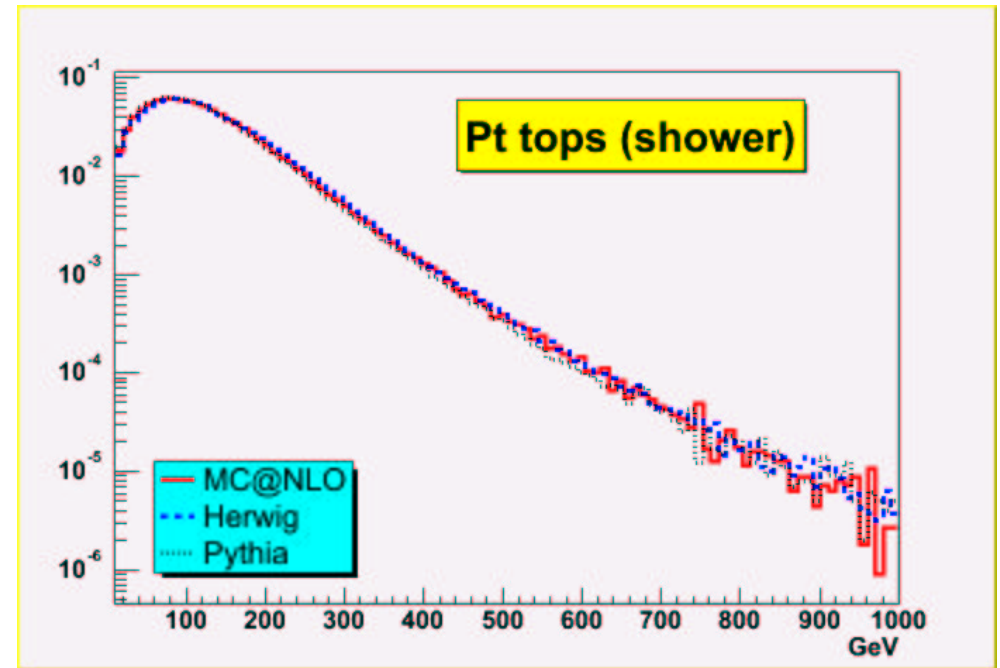
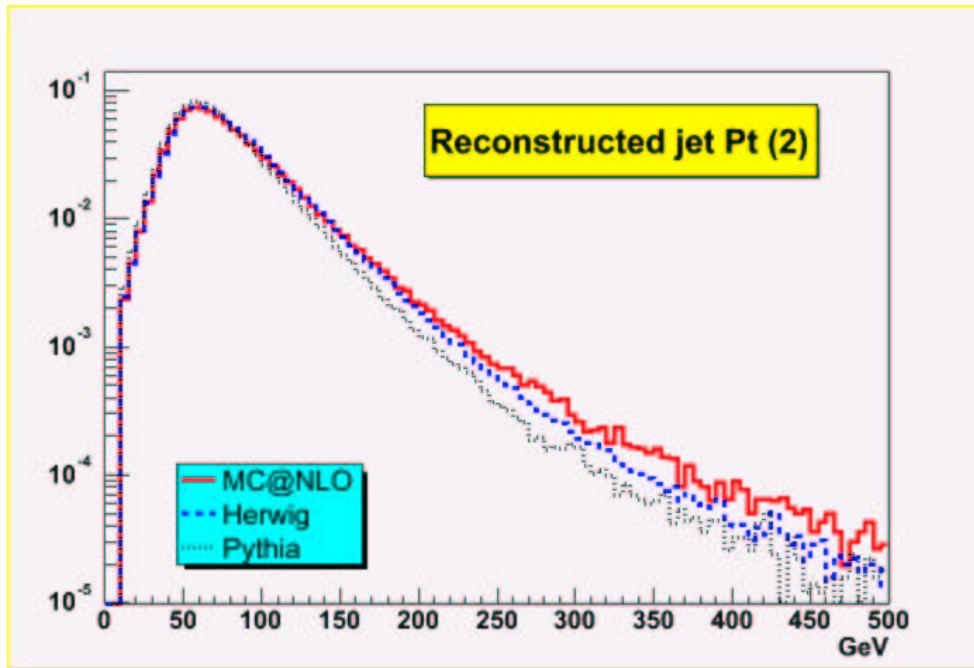


The hard-emission region is basically void in Herwig and Pythia. Furthermore, *all* emissions in Pythia are much softer than in Herwig, leading to a vastly different prediction for the peak of the cross section

Plots: S. Bentvelsen

- This is not peculiar to  $t\bar{t}$  production.  
See [hep-ph/0403100](https://arxiv.org/abs/hep-ph/0403100) for Higgs  $p_T$  spectrum

# A case study: $t\bar{t}$ at LHC II



For certain variables, the agreement is definitely better, since they are dominated by the  $2 \rightarrow 2$  kinematics of the hard process at the LO

Plots: S. Bentvelsen

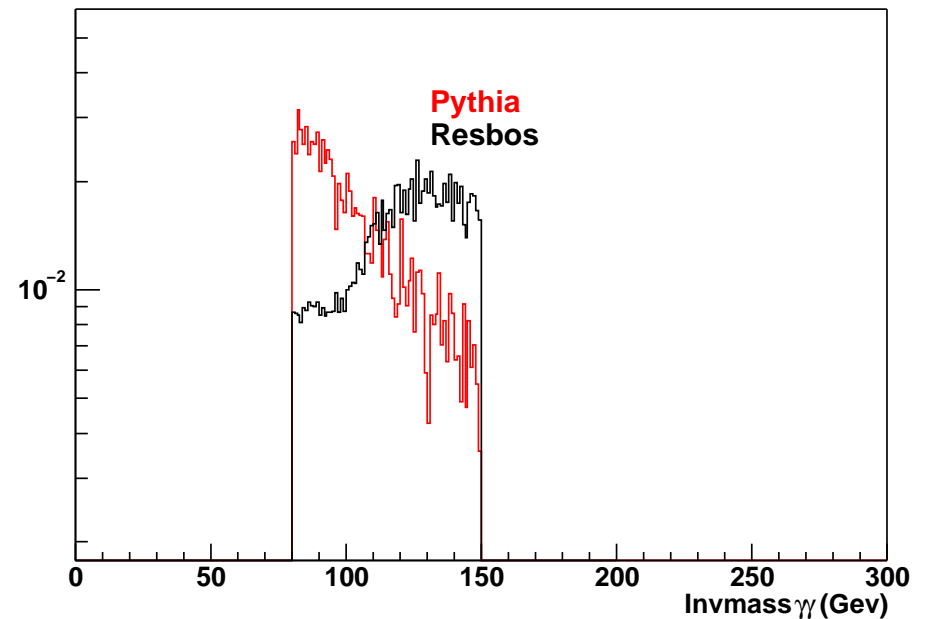
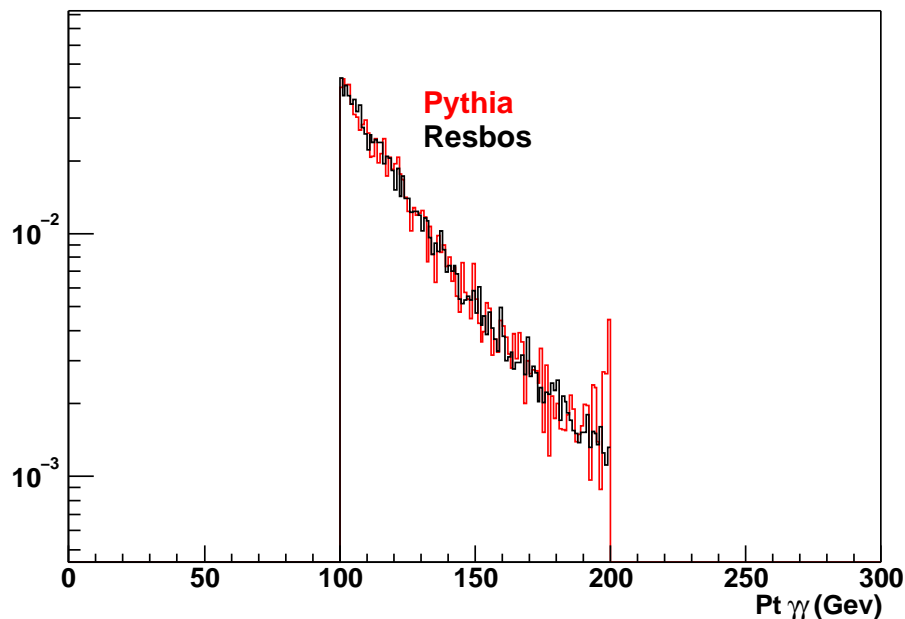
⇒ Multivariate analyses will lead to different results depending on the MC used



# Is reweighting a viable solution?

A common and rather naive practice is that of multiplying the standard MC results by the fully-inclusive K factors

A more sophisticated procedure selects an observable  $O$  for which a resummed and/or fixed-order result is available, and reweights in bins of  $O$  (see e.g. hep-ph/0402218)

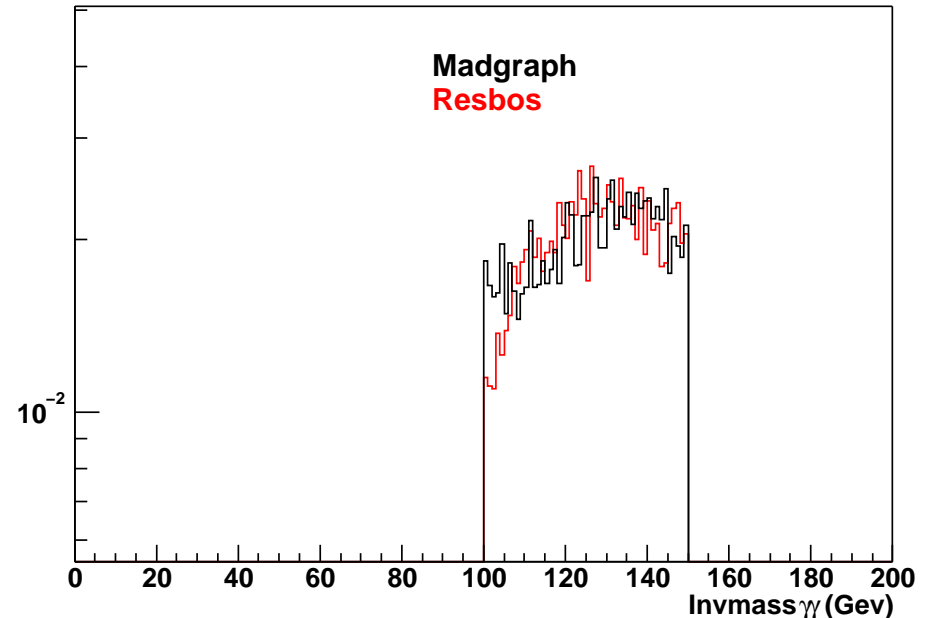
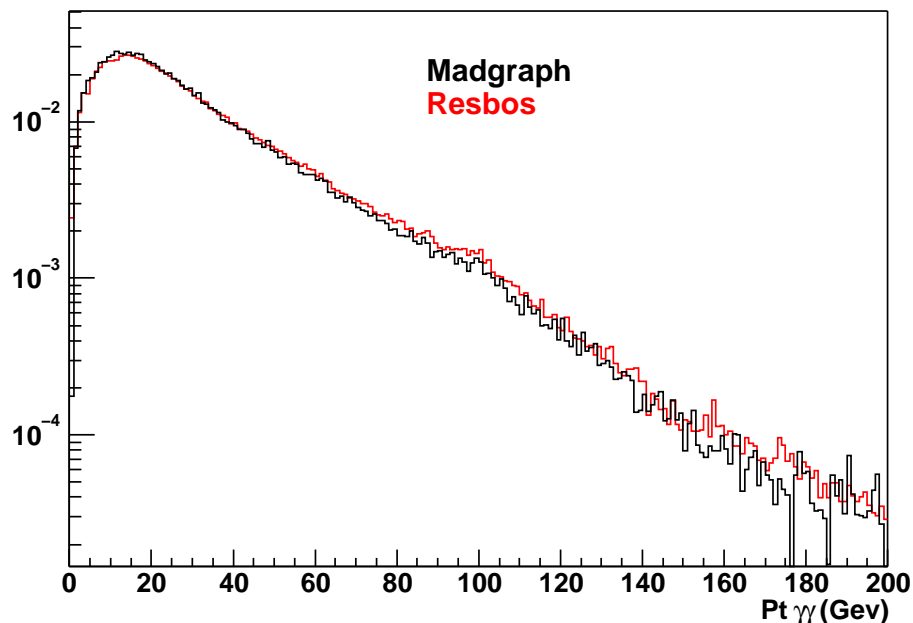


Plots: B. Mellado, Y. Fang

After reweighting  $p_T^{(\gamma\gamma)}$  for  $80 < M^{(\gamma\gamma)} < 150$  GeV in  $pp \rightarrow \gamma\gamma$  production, the result for the  $M^{(\gamma\gamma)}$  distribution is still disappointing

# Reweighting is not an exact procedure

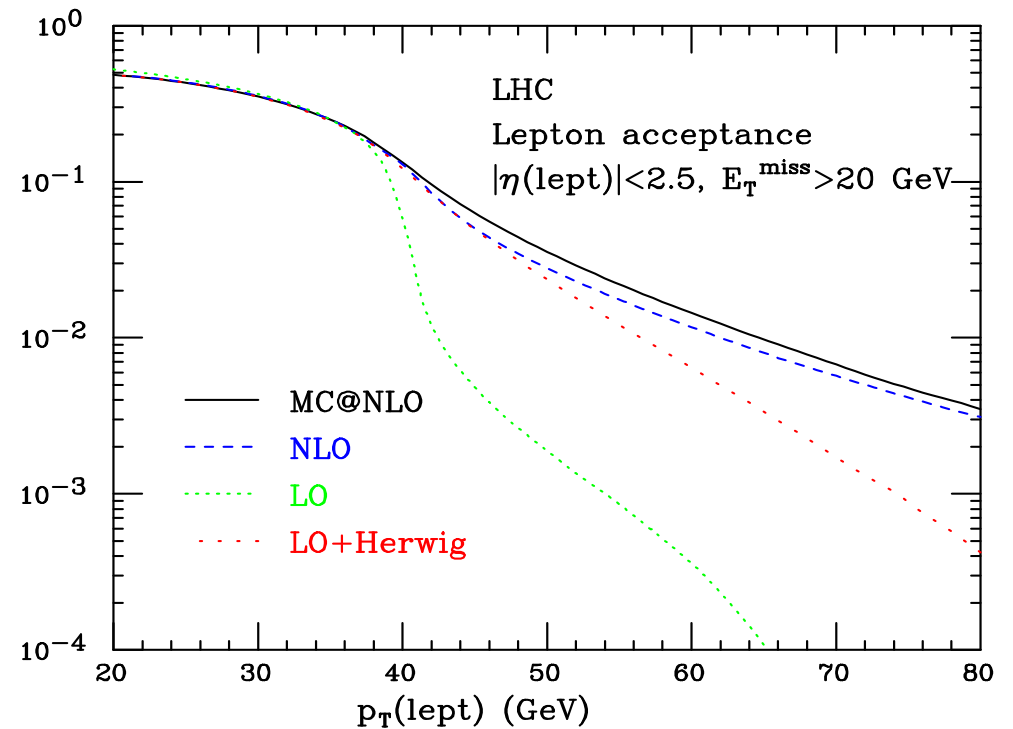
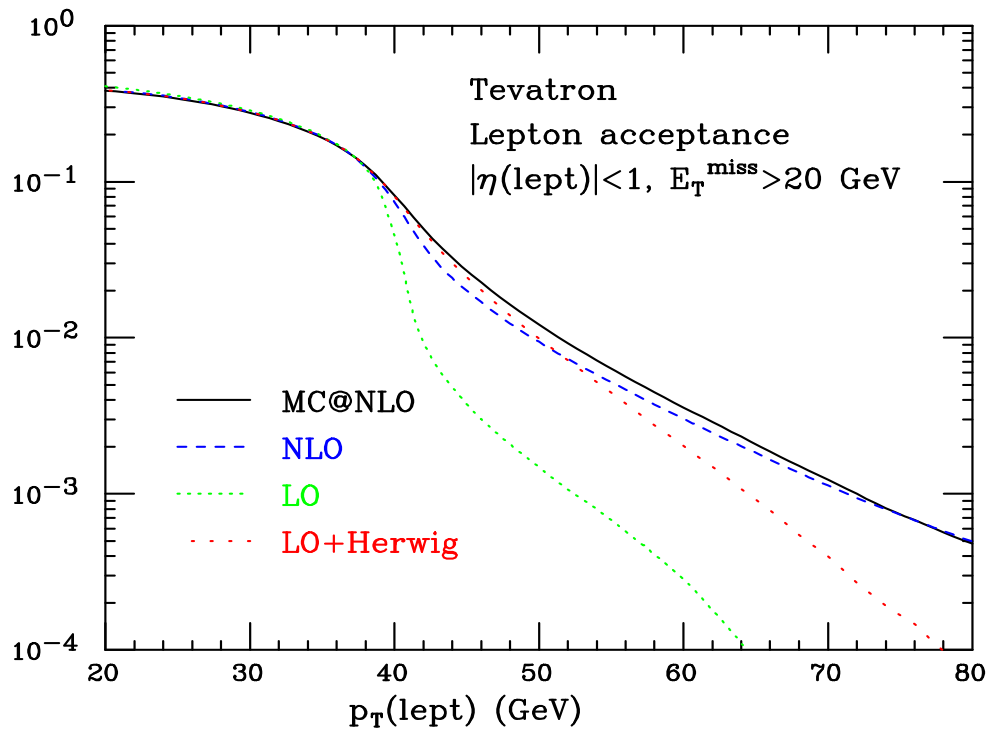
After reweighting  $p_T^{(\gamma\gamma)}$  as predicted by MadGraph for  $100 < M^{(\gamma\gamma)} < 150$  GeV, the  $M^{(\gamma\gamma)}$  distributions are considerably closer



Plots: B. Mellado, Y. Fang

- The results are difficult to predict for the variables not directly involved in the reweighting
- It seems unlikely to get sensible results if the reweighting function is not flat  
 $\Leftrightarrow$  there must be decent agreement between the reweighting and the reweighted kinematics

# W production acceptances



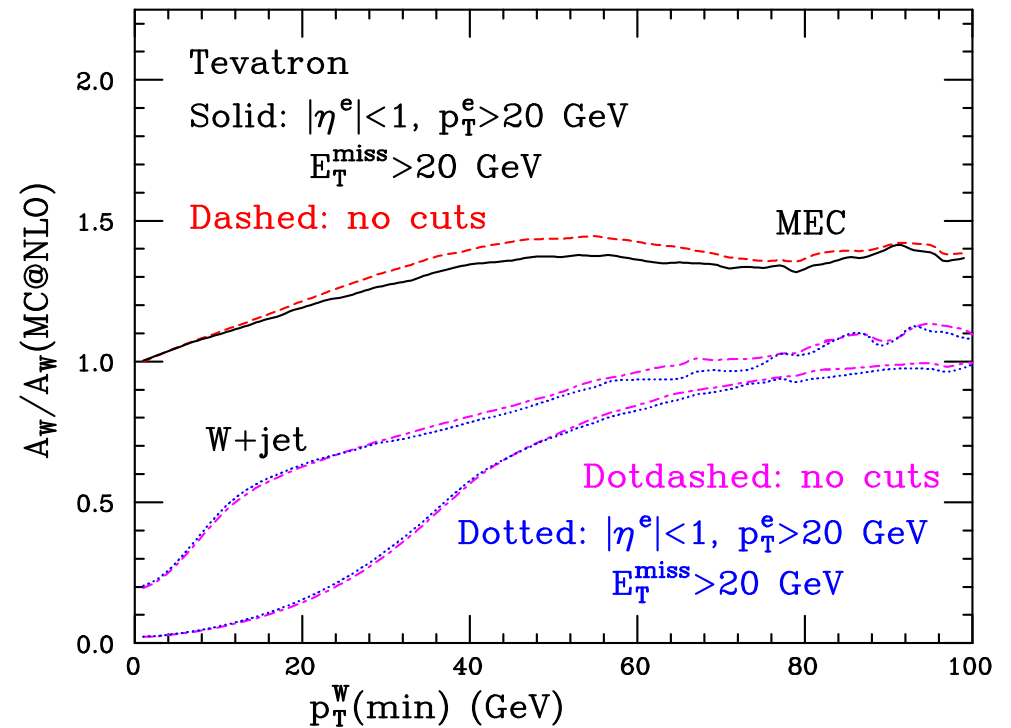
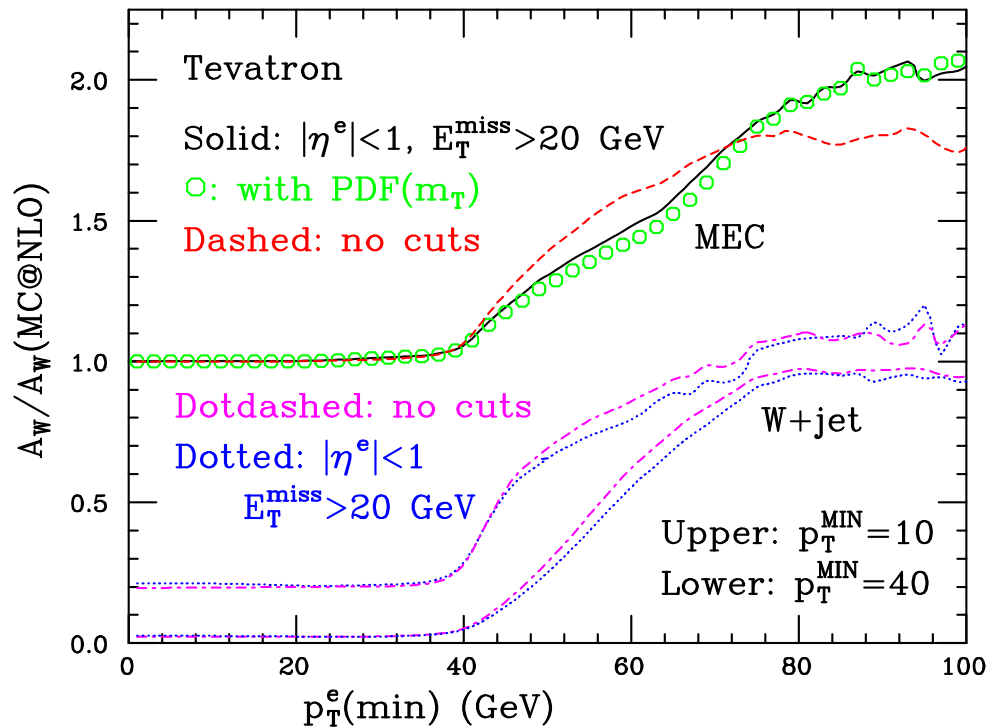
Plots: SF&MLM, hep-ph/0405130

Although MC@NLO uses HERWIG for showering, the hard matrix elements play a dominant role when moving towards phase-space regions dominated by hard emissions

⇒ If these regions are relevant to your favourite analysis, you better use an NLOwPS such as MC@NLO

Why not Matrix Element Corrections?

# MC@NLO vs MEC in $W$ acceptance computations



- ◆ MEC make use of *same real* matrix elements which enter NLO computations. What is the proper normalization in the computation of acceptances?
- ◆ If one uses LO, there is disagreement at high  $p_T$ . If one uses NLO, the disagreement is at low  $p_T$
- Old-fashioned MEC can't give sensible predictions for the entire  $p_T$  range: there are kinematical distortions (true for any process)

# Expect more progress

- ◆ NLOwPS without negative weights (Nason)
  - Move hardest emission up the shower, exponentiate full real corrections
  - Potentially large beyond-NLO spurious contributions – need to check
- ◆ New Pythia showers (Sjöstrand & Skands)
  - Ordered in  $p_T$  rather than in  $Q^2$
  - Identical to UE, closer to exact implementation of color coherence
  - Naturally matching multiple-interaction models (beneficial for UE?)
  - Need to figure out colour correlations; massive testing mandatory
- ◆ C++ stuff (Herwig & Pythia & Sherpa teams)
  - Slower than expected, but it's coming
  - Herwig++ and Sherpa running
  - The final weapon: use hard processes of A, shower of B, and hadronization of C, without changing framework
- ◆ New Pythia and Herwig implementations of UE

# Want to have more details?

## Les Houches Guidebook to Monte Carlo Generators for Hadron Collider Physics

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### Abstract

Recently the collider physics community has seen significant advances in the formalisms and implementations of event generators. This review is a primer of the methods commonly used for the simulation of high energy physics events at particle colliders. We provide brief descriptions, references, and links to the specific computer codes which implement the methods. The aim is to provide an overview of the available tools, allowing the reader to ascertain which tool is best for a particular application, but also making clear the limitations of each tool.

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The Les Houches MC guidebook ([hep-ph/0403045](https://arxiv.org/abs/hep-ph/0403045)) presents short introductions to the topics of perturbative QCD relevant to MC simulations, and an updated list of available MC's

# 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

- 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 and unphysical parameters

The community is responding well to the challenges of LHC – however, there will be no real progress until these new tools will be routinely used by experiments. The role of Tevatron will be especially crucial