Stefano Frixione

MC@NLO

Theory for Experimentalists, Durham, 20/2/2008

The problem

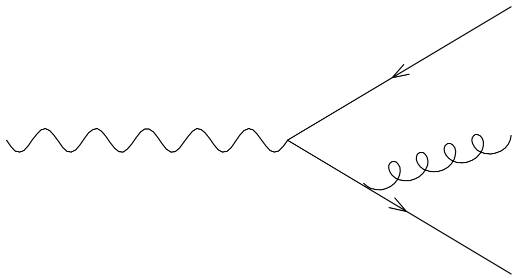
- A lot of physics at the LHC will involve many-jet events, and processes with large K factors

- Monte Carlos cannot give sensible descriptions of many-jet events, and cannot compute K factors

- Although Monte Carlos *must not* be seen as discovery tools, these issues must be addressed for a good understanding of LHC physics

A 30'' guide to Monte Carlos

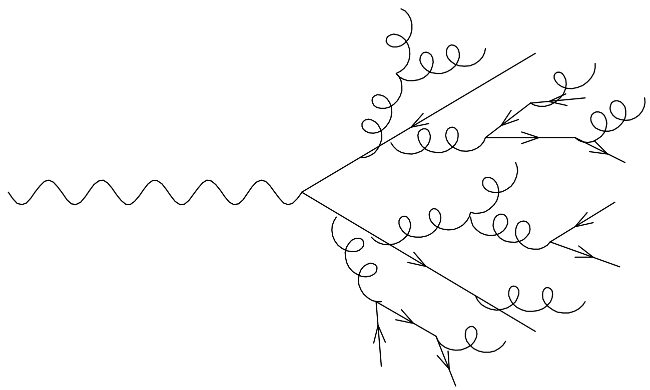
Key observation: collinear emissions factorize



$$d\sigma_{q\bar{q}g} \xrightarrow{t\to 0} d\sigma_{q\bar{q}} \times \frac{\alpha_S}{2\pi}\frac{dt}{t}P_{qq}(z)dz\frac{d\varphi}{2\pi}$$

$$t = (p_q + p_g)^2\,, \qquad z = E_q/(E_q + E_g)$$

Obviously, the process can be iterated as many times as one wants $\longrightarrow$ parton shower; emissions are exponentiated into a Sudakov form factor



- Shower resums leading logarithmic contributions
- The cross sections are always positive (and at leading order)
- Large final-state multiplicities: fully realistic description of the collision process, including hadronization and underlying event
- Monte Carlos differ in the choice of *shower variables*: z, t

Double logs

QCD has soft divergences. In MC's they are easy to locate:

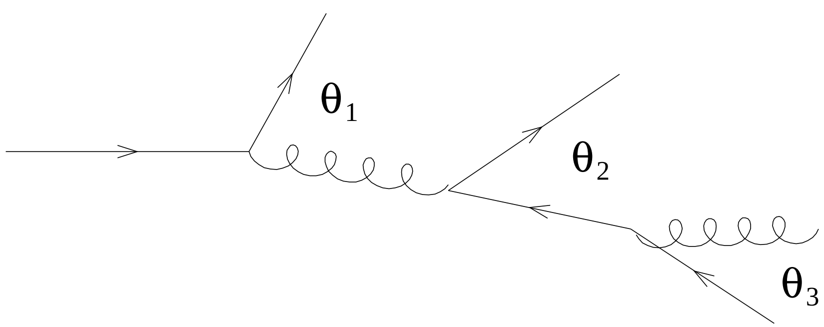
$$z \to 1 \qquad \Longrightarrow \qquad P_{qq},\ P_{gg} \sim \frac{1}{1-z}$$

The choice of shower variables affects the double-log structure

$$t = z(1-z)\theta^2 E^2 \quad (\text{virtuality}) \qquad \Longrightarrow \qquad \frac{1}{2}\log^2\frac{t}{E^2}$$

$$t = z^2(1-z)^2\theta^2 E^2 \quad (p_T^2) \qquad \Longrightarrow \qquad \log^2\frac{t}{E^2}$$

$$t = \theta^2 E^2 \quad (\text{angle}) \qquad \Longrightarrow \qquad \log\frac{t}{\Lambda}\log\frac{E}{\Lambda}$$



The choice that respects colour coherence is angular ordering (Mueller), as in HERWIG:

$$\theta_1 > \theta_2 > \theta_3$$

Summary on Parton Shower Monte Carlos

Based on simple ideas with profound implications. Very flexible, essential tools for experimental physics. But:

- Each emission in a shower is based on a collinear approximation
- At the LHC, there is a lot of energy available: very easy to get large-angle, large-energy emissions
- The larger the angle of emission, the less accurate the MC prediction

Is predictivity an issue?

To a large extent, it didn't use to be: MC's were as good as their ability to fit the data*

So MC's with a lot of parameters are likely to fit the data – which is what made most theorists proud of not knowing anything about MC's

- There are large uncertainties in QCD: one can go way too far beyond limits of applicability of the MC, without noticing it
- To stretch the theory to fit data may hide some interesting unknown physics

We really don't know what will happen at the LHC: predictivity is an (important) issue**. Unaware theorists not really ashamed, but less proud

* Data have been instrumental in forcing MC's to improve/upgrade: colour coherence, b physics are major examples

** MC's must still be able to fit the data to permit unbiased data analysis

How to improve Monte Carlos?

The key issue is to go beyond the collinear approximation

$\Longrightarrow$ use exact matrix elements of order higher than leading

Fixed-order vs MC's

- Fixed-order results: reliable predictions for total rates and large-p_T tails for inclusive quantities

  "Rare" events

- Parton Shower Monte Carlos: predictions for peak regions and large-multiplicity final states

  Most probable events

The complementarity of the two approaches renders their merging into a single formalism particularly desirable and challenging

We have basically learned how to achieve this in the past two-three years

How to improve Monte Carlos?

The key issue is to go beyond the collinear approximation*

$\Longrightarrow$ use exact matrix elements of order higher than leading

Which ones?

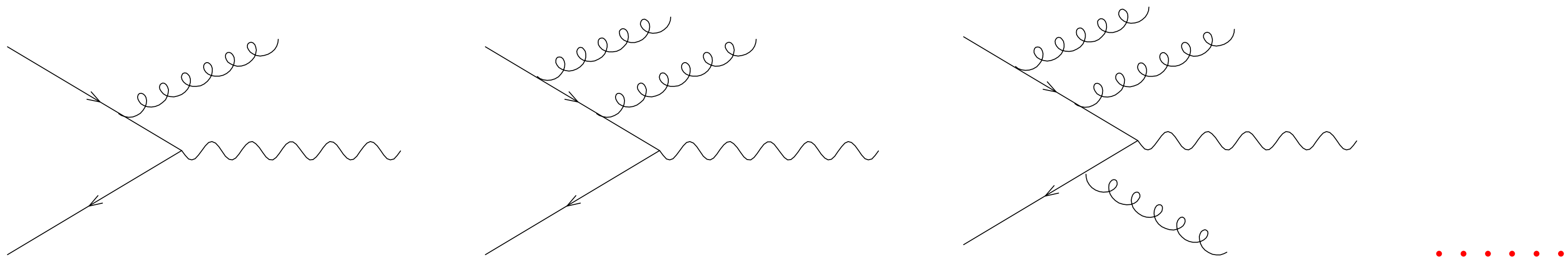
There are two possible choices, that lead to two vastly different strategies:

- Matrix Element Corrections $\longrightarrow$ tree level
- NLOwPS $\longrightarrow$ tree level and loop

* 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

Matrix Element Corrections

Compute (exactly) as many as possible real emission diagrams before starting the shower. Example: W production



Problems

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

Solution

$\longrightarrow$ Catani, Krauss, Kuhn, Webber (2001), Lonnblad (2002), Mangano (2005)

How to achieve MEC

- Preliminary step: compute the real matrix elements

  Non trivial for high-multiplicities. Problem now fully solved and highly automatized (`AcerMC`, `ALPGEN`, `AMEGIC++`, `CompHEP`, `Grace`, `MadEvent`)

- The strategy: apply a cut δ_{sep} on matrix elements to avoid divergences

  For a fixed multiplicity n, this implies a large, unphysical δ_{sep} dependence

$$\sigma_n \sim \alpha_S^{n-2} \sum_k a_k \alpha_S^k \log^{2k} \delta_{sep}$$

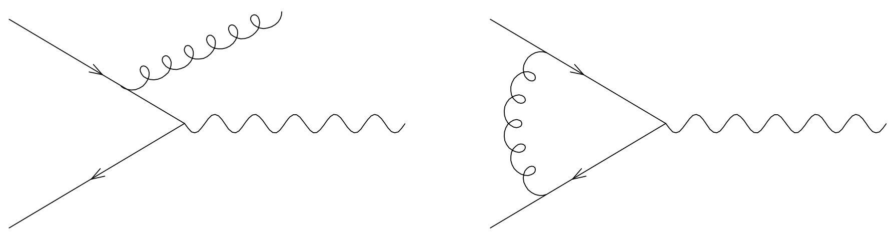
Then reweight ME's and modify the shower to eliminate or reduce the δ_{sep} dependence

  Following CKKW, one gets

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

NLOwPS

Compute all the NLO diagrams (and only those) before starting the shower.
Example: W production



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Problems

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

Solution

$\longrightarrow$

Proposals for NLOwPS's

- First working hadronic code (Z): Φ-veto (Dobbs, 2001)
- First correct general solution: MC@NLO (Frixione, Webber, 2002)
- Automated computations of ME's: grcNLO (GRACE group, 2003)
- Absence of negative weights (Nason, 2004; Frixione, Nason, Oleari, 2007) – POWHEG
- Showers with high log accuracy in ϕ_6^3 (Collins, Zu, 2002–2004)
- Proposals for $e^+e^- \to jets$ (Soper, Krämer, Nagy, 2003–2006)
- Shower and matching with QCD antennae (Giele, Kosower, Skands 2007) – VINCIA
- Within Soft Collinear Effective Theory (Bauer, Schwartz, 2006)
- With analytic showers (Bauer, Tackmann, Thaler, 2008) – GenEvA

There has been also a substantial amount of activity on alternative formulations of basic QCD showers, which may (or may not) help the matching with NLO matrix elements

On NLOwPS

- A proper NLOwPS is a *formalism*, not a code. It is a solution of the theoretical problem of matching NLO results with Monte Carlos
- That said, in order to prove that such solution works, implementation in a code is mandatory. Note that an NLOwPS may not work *also* because of practical problems (such as numerical instabilities)

So far, MC@NLO and POWHEG are the only NLOwPS's which have fully made these two steps in the context of hadronic collisions. For MC@NLO:

- Several processes implemented: W, Z, H, $l\bar{l}$, $l\nu$, $b\bar{b}$, $t\bar{t}$, HW, HZ, single top, W^+W^-, ZZ, WZ; most of these now include decay correlations
- Used for some $b\bar{b}$ and $t\bar{t}$ analysis at Tevatron, and for several simulations at LHC
- Lot of work in progress (eg, dijet, Higgs in VBF, Wt, PYTHIA, HERWIG++)

POWHEG features ZZ and $Q\bar{Q}$ production so far. Good agreement with MC@NLO in spite of lack of soft showers

NLOwPS vs Matrix Element Corrections

NLOwPS are vastly different from MEC. MEC lack virtual corrections

This forces the use of an unphysical cutoff δ_{sep} in MEC, upon which physical observables depend $\longrightarrow$ matching systematics

MC@NLO is better than MEC since:

+ There is no δ_{sep} dependence (i.e., no matching systematics)
+ The computation of total rates is meaningful and reliable

MC@NLO is worse than MEC since:

− The number of hard legs is smaller

■ The days of the universal tools are over. Choose the one that best suits your analysis. Typically: small/large number of *extra* legs $\Longrightarrow$ MC@NLO/MEC

Why NLO corrections?

- NLOwPS's are the only way in which K-factors can be embedded into MC's (no rescaling please!)
- The scale dependence of observables can be computed
- Realistic hadronization for NLO-accurate predictions
- Allow a fully-consistent determination of PDF uncertainties (PDF with errors are NLO fits), and of PDFs themselves
- Non-trivial dynamics beyond LO ($t-\bar{t}$ asymmetry, FCR vs FEX vs GSP in $b\bar{b}$, $qg \to Wq$, $Wt \leftrightarrow t\bar{t}$ interference, ...)

MC@NLO 3.3 [hep-ph/0612272]

IPROC	IV	IL_1	IL_2	Spin	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		7	7	×	$H_1H_2 \to t\bar{t} + X$
–1706		i	j	✓	$H_1H_2 \to (t \to) b l_i^+ \nu_i (\bar{t} \to) \bar{b} l_j^- \bar{\nu}_j + X$
–2000–IC		7		×	$H_1H_2 \to t/\bar{t} + X$
–2000–IC		i		✓	$H_1H_2 \to (t \to) b l_i^+ \nu_i / (\bar{t} \to) \bar{b} l_i^- \bar{\nu}_i + X$
–2001–IC		7		×	$H_1H_2 \to \bar{t} + X$
–2001–IC		i		✓	$H_1H_2 \to (\bar{t} \to) \bar{b} l_i^- \bar{\nu}_i + X$
–2004–IC		7		×	$H_1H_2 \to t + X$
–2004–IC		i		✓	$H_1H_2 \to (t \to) b l_i^+ \nu_i + X$
–2600–ID	1	7		×	$H_1H_2 \to H^0 W^+ + X$
–2600–ID	1	i		✓	$H_1H_2 \to H^0 (W^+ \to) l_i^+ \nu_i + X$
–2600–ID	-1	7		×	$H_1H_2 \to H^0 W^- + X$
–2600–ID	-1	i		✓	$H_1H_2 \to H^0 (W^- \to) l_i^- \bar{\nu}_i + X$
–2700–ID	0	7		×	$H_1H_2 \to H^0 Z + X$
–2700–ID	0	i		✓	$H_1H_2 \to H^0 (Z \to) l_i \bar{l}_i + X$
–2850		7	7	×	$H_1H_2 \to W^+W^- + X$
–2850		i	j	✓	$H_1H_2 \to (W^+ \to) l_i^+ \nu_i (W^- \to) l_j^- \bar{\nu}_j + X$
–2860		7	7	×	$H_1H_2 \to Z^0Z^0 + X$
–2870		7	7	×	$H_1H_2 \to W^+Z^0 + X$
–2880		7	7	×	$H_1H_2 \to W^-Z^0 + X$

Recent activities:

- Lepton spin correlations in $t\bar{t}$ and single-top production released with v3.3
- Hadron spin correlations in $t\bar{t}$ now into ATLAS and CMS software (v3.31)
- W and Z production with interface to HERWIG++
- Early stage of interface to PYTHIA
- Wt is now completed

http://www.hep.phy.cam.ac.uk/theory/webber/MCatNLO

Running MC@NLO

NLO code $\longrightarrow$ Event file $\longrightarrow$ MC code

- NLO code: integrates and unweights the matrix elements
- Event file: a list of hard events, i.e. the kinematics configurations emerging from hard subprocesses (typically, $2 \to 2$ and $2 \to 3$)
- MC code: HERWIG, which reads the hard events and showers them

The flowchart is the same as in MEC-based simulations. Features:

- Less than 1 hour for $1/2$ million $t\bar{t}$ hard events on my (2003) laptop
- Unweighting efficiency: 10-40%
- Events have weights ± 1

Negative weights

- Why are they around?

  Exact quantum mechanics computations feature interference phenomena, whose contributions don't have a definite sign. The presence of contributions of negative sign to the cross sections prevents us from having *only* $+1$ weights

- What's the difference wrt NLO?

  At the NLO, the negative-only weight distribution is divergent, while it is finite in MC@NLO. Unweighted event generation can only be achieved in MC@NLO

- Can I throw them away in MC@NLO?

  No, you can't: they are necessary in order to obtain the exact NLO results for total rates, and for differential distributions where relevant

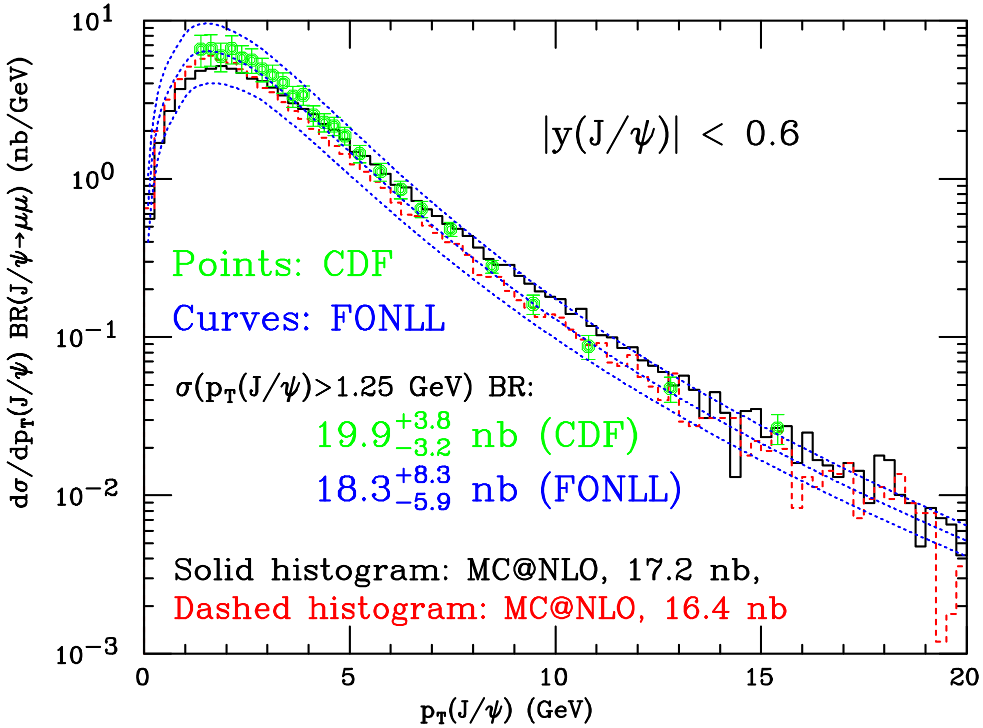
- How do I have to use them?

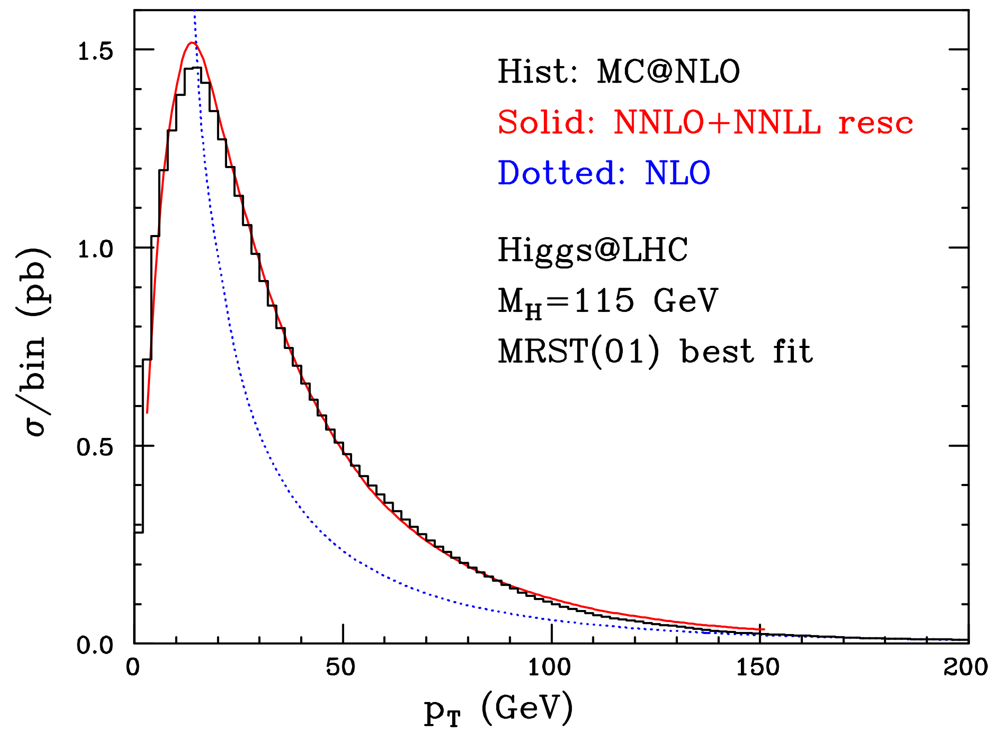
  Just add -1 to *(i.e. subtract* $+1$ *from)* the histograms of physical observables. For geometric properties, treat them as you treat the positive weights

The only implication of negative weights is that you have to run a bit longer to obtain the same nominal accuracy – and in b physics you actually have to run *less*

WHY NLO:
EXAMPLES WITH MC@NLO

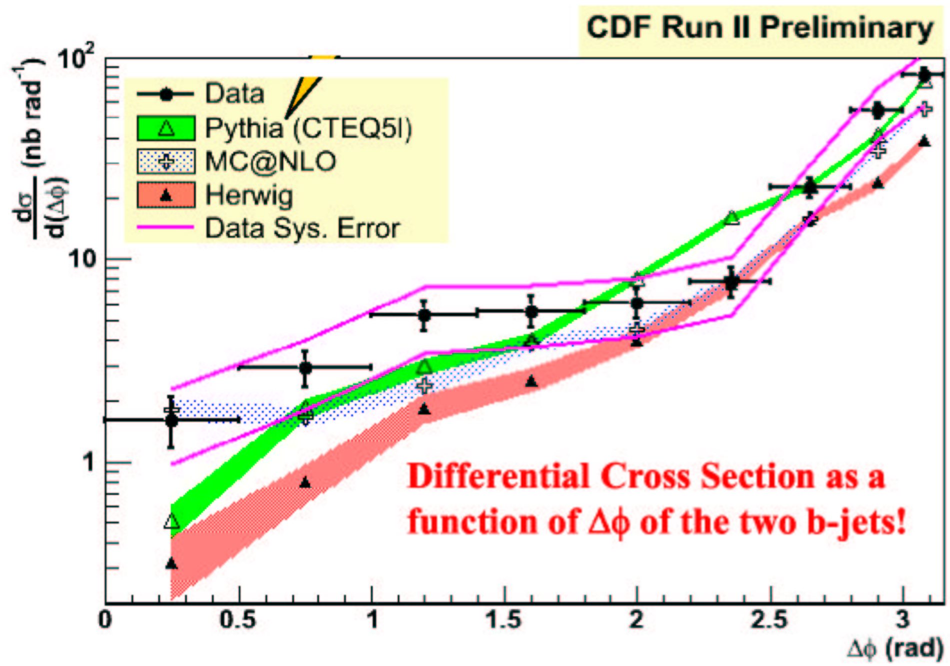
MC@NLO vs analytical results

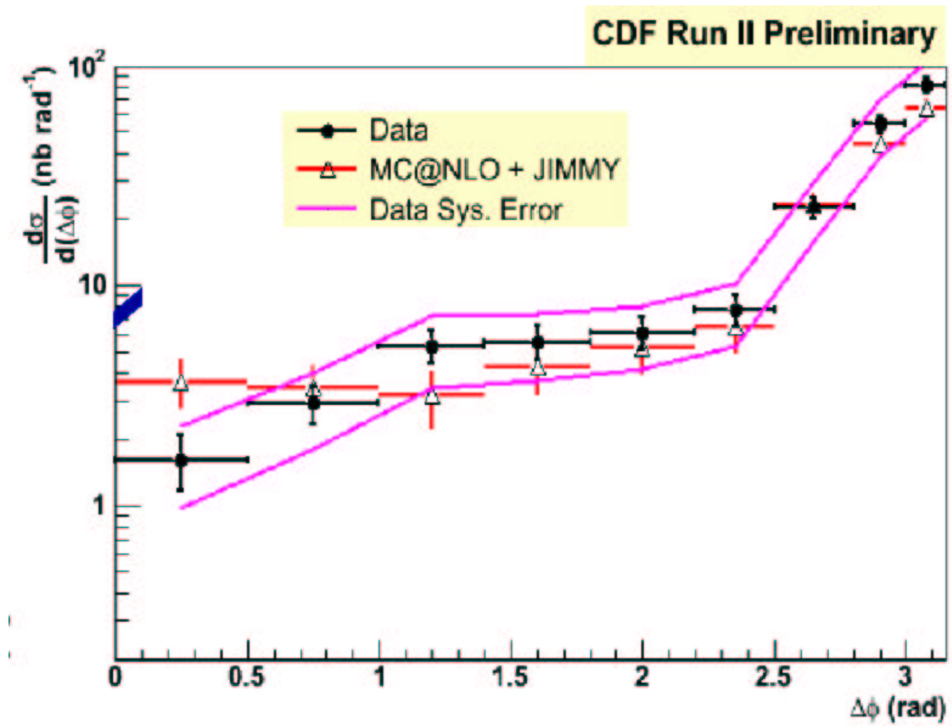




- Get right shapes *and* rates
- Note: analytical resummations are *formally* more accurate: Cacciari, Nason (single-inclusive b), Bozzi, Catani, de Florian, Grazzini (Higgs)
- MC@NLO thus effectively allows one to perform high-accuracy computations in a realistic environment (as complicated as detector simulations)

$b\bar{b}$ correlations





- These observables are very involved (b-jets at hadron level), and cannot be computed with analytic techniques
- The importance of the underlying event stresses the necessity of embedding a *precise* computation into a Monte Carlo framework, as done in MC@NLO

W production acceptances

	LO		LO+HW	NLO		MC@NLO
Cuts A	0.5249	$\xrightarrow{-7.7\%}$	0.4843	0.4771	$\xrightarrow{+1.5\%}$	0.4845
	↓5.4%			↓7.0%		↓6.3%
Cuts A, no spin	0.5535			0.5104		0.5151
Cuts B	0.0585	$\xrightarrow{+208\%}$	0.1218	0.1292	$\xrightarrow{+2.9\%}$	0.1329
	↓29%			↓16%		↓18%
Cuts B, no spin	0.0752			0.1504		0.1570

@LHC: Cuts A $\longrightarrow$ $\left|\eta^{(e)}\right| < 2.5$, $p_T^{(e)} > 20$ GeV, $p_T^{(\nu)} > 20$ GeV

Cuts B $\longrightarrow$ $\left|\eta^{(e)}\right| < 2.5$, $p_T^{(e)} > 40$ GeV, $p_T^{(\nu)} > 20$ GeV

- NLO+Shower $\Longrightarrow$ stable results
- Spin correlations are important

Single-top in Wt mode

- As with s- and t-channels, a direct probe of top weak interactions
- A background to $t\bar{t}$ and to $gg \rightarrow H(\rightarrow W^+W^-)$

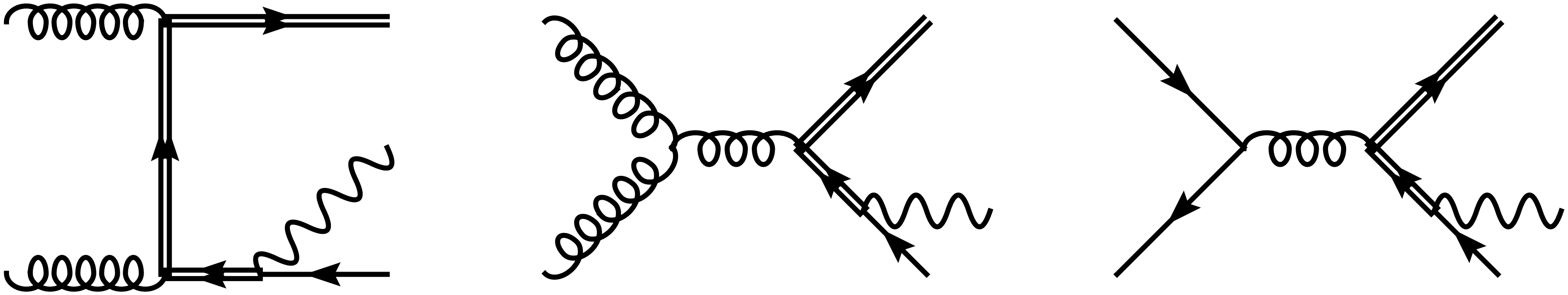
Apart from putting Wt MC predictions on firmer ground, the inclusion of this process into MC@NLO allows one to discuss a very interesting problem

$$
\begin{aligned}
b+g &\longrightarrow t+W \\
b+g &\longrightarrow t+W+g \\
g+g &\longrightarrow t+W+\bar{b} \\
q+\bar{q} &\longrightarrow t+W+\bar{b} \\
b+q &\longrightarrow t+W+q \\
b+\bar{b} &\longrightarrow t+W+\bar{b} \\
b+b &\longrightarrow t+W+b
\end{aligned}
$$

The b's are massless

Troubles...

...are due to (part of) the real corrections



One just can't tell whether these diagrams are relevant to $t\bar{t}$ (with the t decay not drawn) or to Wt production

- $t\bar{t}$ and Wt production *interfere*

This problem has been tackled in many different ways (Kauer, Zeppenfeld; Belyaev, Boos, Dudko; Tait; Campbell, Tramontano; ...)

However, IMHO the *only realistic approaches* are in an NLOwPS context. We have achieved this in MC@NLO. Results will be public in a few weeks

Outlook (for experimenters)

NLOwPS's give more reliable predictions than standard MC's.
They should be seen as default choices, with MC's as backups

- NLOwPS and MEC have complementary advantages
- More partonic processes in hard reactions: *new observable effects*
- No necessity to reweight/rescale: correct K factors included
- Hadronization corrections to NLO observables (jets)
- Another, more solid, way to study systematics: scale variation
- MC@NLO is official software of (some of the) collider experiments. Expect more processes to be implemented in the near future

Most technical obstacles cleared. But it is extremely important that experimenters will extensively test these ideas. This is crucial in order to correct mistakes, identify priorities, and motivate theoretical progress

BACKUP SLIDES

MC@NLO: formalism

Double counting $\Longleftrightarrow$ MC evolution results in spurious NLO terms

$\longrightarrow$ *Eliminate the spurious NLO terms "by hand"*

- The generating functional is

$$\mathcal{F}_{\text{MC@NLO}} = \sum_{ab} \int dx_1\, dx_2\, d\phi_{n+1}\, f_a(x_1) f_b(x_2) \times \Big[\mathcal{F}_{\text{MC}}^{(2\to n+1)} \left(\mathcal{M}_{ab}^{(r)} - \mathcal{M}_{ab}^{(\text{MC})} \right) + \mathcal{F}_{\text{MC}}^{(2\to n)} \left(\mathcal{M}_{ab}^{(b,v,c)} - \mathcal{M}_{ab}^{(c.t.)} + \mathcal{M}_{ab}^{(\text{MC})} \right) \Big]$$

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

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

MC@NLO in a nutshell

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. Implement the NLO matrix elements of your favourite process according to the universal, observable-independent, subtraction-based formalism of SF, Kunszt, Signer (Nucl.Phys.B467(1996)399) for cancelling IR divergences

   This is the only non-trivial step necessary in order to add new processes

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

On step 1: MC counterterms

- An analytic computation is needed for each type of MC branching from a massless leg: there are only two cases!

- Initial-state branchings have been studied in JHEP0206(2002)029 (SF, Webber) and JHEP0308(2003)007 (SF, Nason, Webber)

- Final-state branchings have been studied in JHEP0603(2006)092 (SF, Laenen, Motylinski, Webber)

For each new process, just assemble these pieces into a computer code. No new computation is now required for matching with fortran HERWIG

On MC@NLO code

Time for the inclusion of a new process is spent:

- 80% for the pure-NLO computation
- 15% for MC counterterms and LHI-related code
- 5% debugging

The structure of the MC counterterms is modular

$$\mathcal{M}^{(\mathrm{MC})} = \mathcal{K}^{(\mathrm{MC})} \mathcal{M}^{(b)}$$

Kernels $\mathcal{K}^{(\mathrm{MC})}$ now fully worked out for HERWIG

- Work in progress (Seyi Latunde-Dada) on the computation of $\mathcal{K}^{(\mathrm{MC})}$ for HERWIG++

Basic features

- Inclusive rates accurate to NLO (in α_s)
- More predictive than LO-based MC's (as usual when LO $\longrightarrow$ NLO) for shapes *and* rates
- The above true only for small numbers of extra jets – prefer CKKW-like procedures for many jets
- Tuning is the same as for the MC used for showering (presently only HERWIG) $\Longrightarrow$ smoother version upgrades

The merging of NLOwPS and MEC into a single formalism is feasible.
Some approaches (VINCIA, GenEvA) are constructed with this goal in mind