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Monte Carlos at NLO accuracy

LoopFest V, SLAC, 19/6/2006

Memento

- The most important thing to keep in mind is a simple fact: independently of the implementation, each emission in a shower is based on a collinear approximation
- The larger the angle of emission, the less accurate the MC prediction
- At the LHC, there is a lot of energy available: very easy to get large-angle, large-energy emissions

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

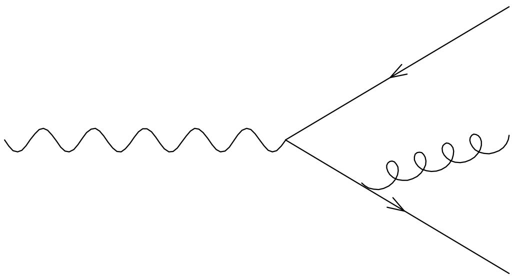
We really don't know what will happen at the LHC: predictivity is an (important) issue**. Unaware theorists not really ashamed, but less proud

* 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

A 30" guide to Monte Carlos

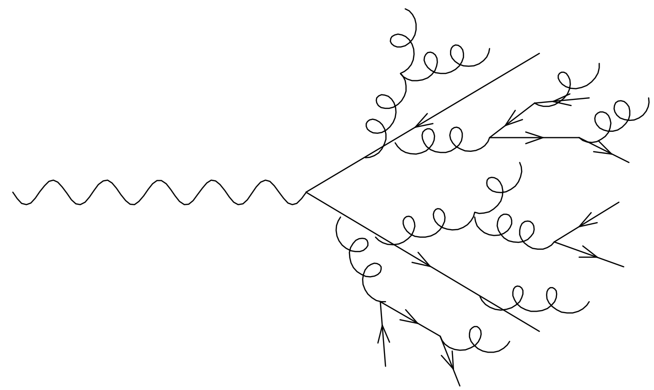
Key observation: collinear emissions factorize



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

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

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

Showering

It's all done through

$$\Delta(t_1, t_2) = \exp\left(-\frac{1}{2\pi}\int_{t_1}^{t_2}\frac{dt}{t}\int_{\varepsilon(t)}^{1-\varepsilon(t)} dz\,\alpha_S(z(1-z)t)P(z)\right)$$

0. Compute the LO cross section. Colour connections determine the initial value of $t = t_{ini}$ for each leg. The lowest value $t = t_0$ is a free parameter

1. With r a random number, solve for t

$$\Delta(t, t_{ini}) = r\,, \qquad t < t_{ini}$$

2. If $t < t_0$, no emission and exit; else, get a z according to $P(z)$, generate an emission (*a branching*) with (z, t), set $t_{ini} = t$, and go to 1.

$\Delta(t_1, t_2)$ is the no-branching probability for $t_1 < t < t_2$

Double logs

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

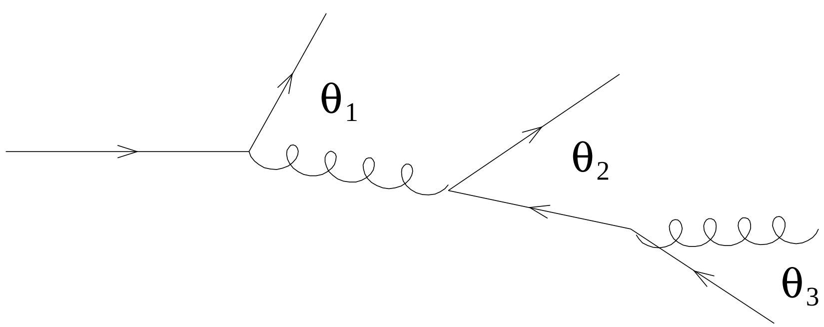
$$z \to 1 \qquad \Longrightarrow \qquad P_{qq},\ P_{gg} \sim \frac{1}{1-z}$$

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:

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

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

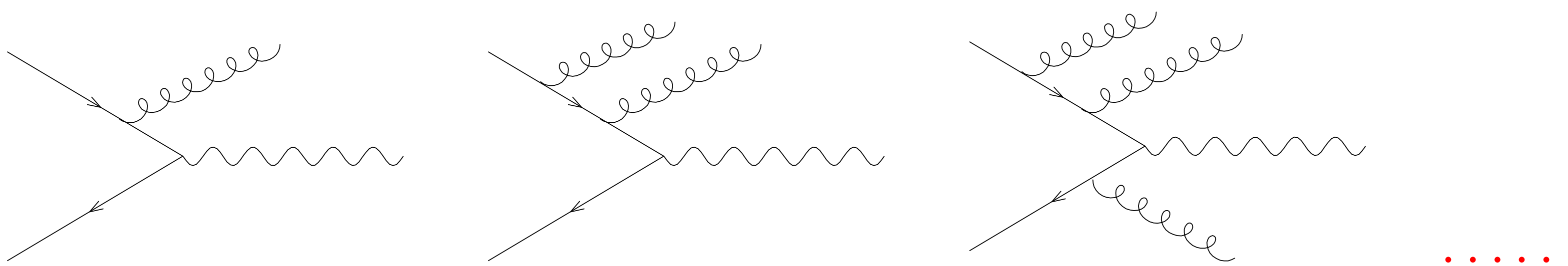
Which ones?

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

- Matrix Element Corrections
- NLOwPS

Matrix Element Corrections

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



Problems

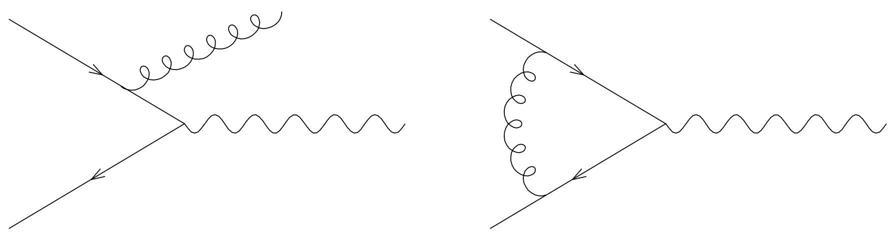
- Double counting (the shower can generate the same diagrams)
- The diagrams are divergent

Solution

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

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

$\longrightarrow$ This talk

NLOwPS versus MEC

- Why is the definition of NLOwPS's 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 δ_{sep}. This must be so, since only loop diagrams can cancel the divergences of real matrix elements

NLOwPS's are better than MEC since:

+ There is no δ_{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

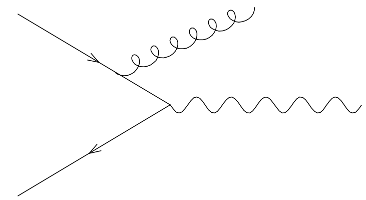
− Computations are more complicated

NLO and MC computations

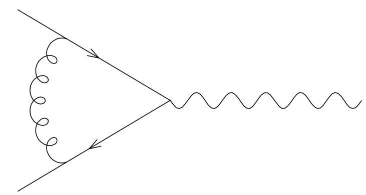
NLO cross section (based on subtraction)

$$\left(\frac{d\sigma}{dO}\right)_{subt} = \sum_{ab} \int dx_1\, dx_2\, d\phi_{n+1}\, f_a(x_1) f_b(x_2) \times$$

$$\Big[\delta(O - O(2 \to n+1))\mathcal{M}_{ab}^{(r)} + \longleftarrow$$



$$\delta(O - O(2 \to n))\left(\mathcal{M}_{ab}^{(b,v,c)} - \mathcal{M}_{ab}^{(c.t.)}\right)\Big] \longleftarrow$$



MC

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

- Matrix elements $\longrightarrow$ normalization, hard kinematic configurations
- δ-functions, $\mathcal{F}_{\mathsf{MC}}^{(2\to n)} \equiv$ showers $\longrightarrow$ observable final states

NLO + MC $\longrightarrow$ NLOwPS?

Naive first try: use the NLO kinematic configurations as initial conditions for showers, rather than for directly computing the observables

- $\delta(O - O(2 \to n)) \longrightarrow$ start the MC with n "hard" emissions: $\mathcal{F}_{\mathrm{MC}}^{(2\to n)}$
- $\delta(O - O(2 \to n+1)) \longrightarrow$ start the MC with $n+1$ "hard" emission: $\mathcal{F}_{\mathrm{MC}}^{(2\to n+1)}$

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

It doesn't work:

- Cancellations between $2 \to n+1$ and $2 \to n$ contributions occur after the shower: hopeless from the practical point of view; and, unweighting is impossible
- $(d\sigma/dO)_{naive} - (d\sigma/dO)_{NLO} = \mathcal{O}(\alpha_S)$. In words: double counting

Solution: MC@NLO (SF, Webber (2002))

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

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

- The generating functional is

$$\mathcal{F}_{\text{MC@NLO}} = \sum_{ab} \int dx_1\, dx_2\, d\phi_{n+1}\, f_a(x_1) f_b(x_2) \times$$

$$\Big[\mathcal{F}_{\text{MC}}^{(2\to n+1)} \left(\mathcal{M}_{ab}^{(r)} - \mathcal{M}_{ab}^{(\text{MC})}\right) +$$

$$\mathcal{F}_{\text{MC}}^{(2\to n)} \left(\mathcal{M}_{ab}^{(b,v,c)} - \mathcal{M}_{ab}^{(c.t.)} + \mathcal{M}_{ab}^{(\text{MC})}\right)\Big]$$

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

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

On 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 required

Difficulties

Apart from conceptual problems, there are numerous technical obstacles that must be cleared for the implementation of MC@NLO. Examples are:

- QCD has soft *and* collinear singularities. In the case of initial state emissions, the hard $2 \to n$ processes that factorize have *different kinematics* in the soft and the two collinear limits. But there is only one

  $$\mathcal{F}_{\mathrm{MC}}^{(2\to n)}$$

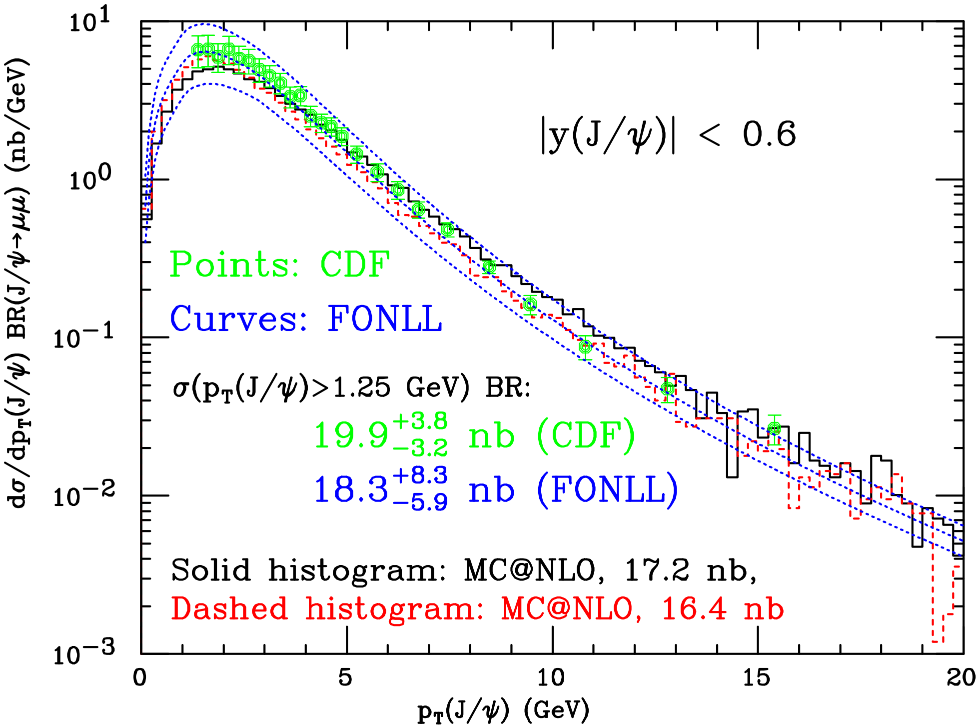
  functional generator, therefore the hard configuration *must be unique*

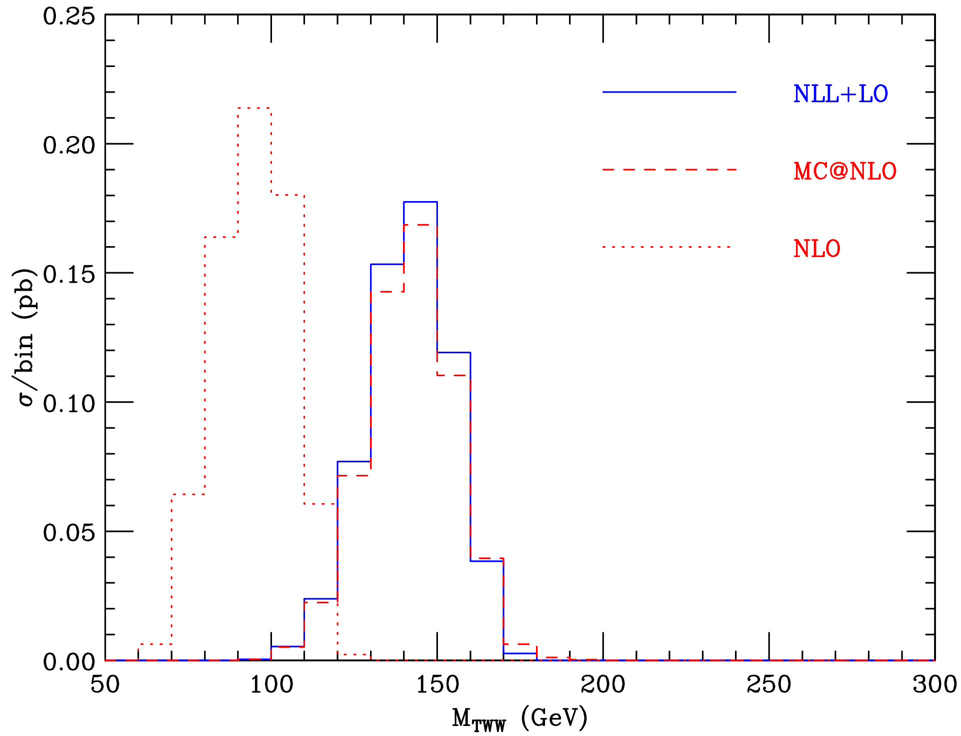
- The computation of the MC counterterms

  $$\mathcal{M}_{ab}^{(\mathrm{MC})}$$

  requires a deep knowledge of MC implementation details. The *shower variables* have to be expressed in terms of the *phase-space variables* ϕ_{n+1} used in the NLO computation

MC@NLO vs analytical resummations



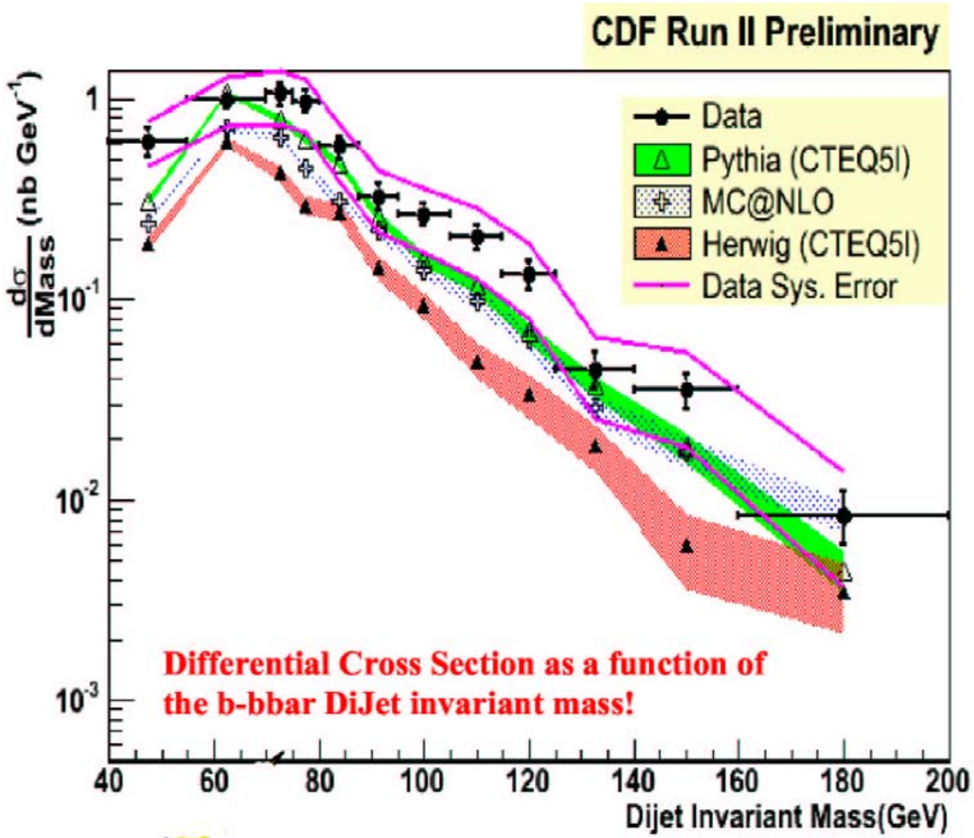


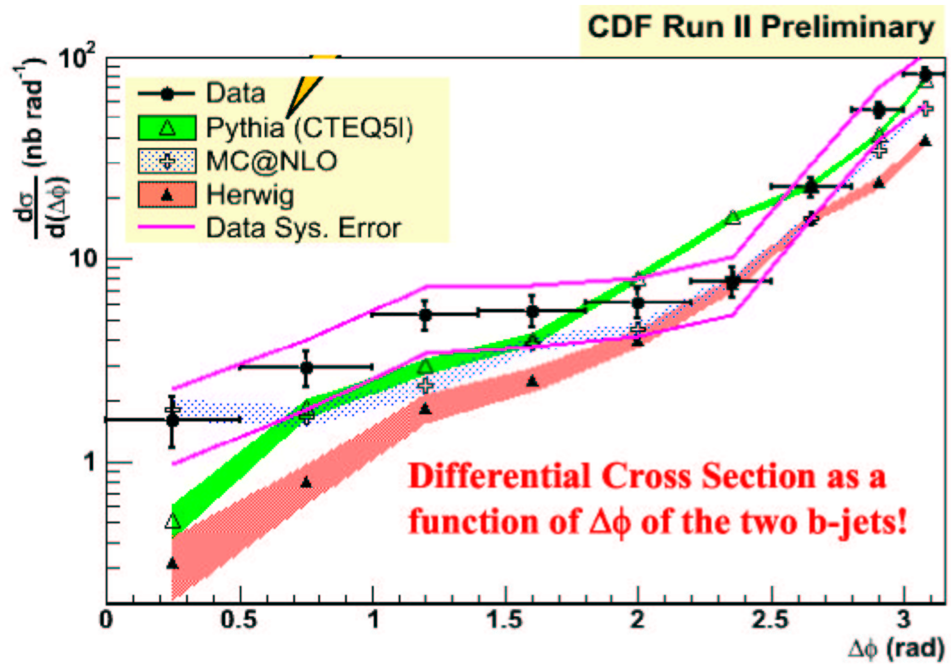
Cacciari, Mangano, Nason, Ridolfi, SF

Grazzini

- Highly non-trivial test (of both computations) for *shapes* and *rates* !
- Best-ever agreement with single-inclusive b data at the Tevatron
- Involved cuts in the definition of M_T: $\Delta\phi_{l^+l^-} < \pi/4$, $M_{l^+l^-} > 35$ GeV, $p_{Tmin}^{(l^+,l^-)} > 25$ GeV, $35 < p_{Tmax}^{(l^+,l^-)} < 50$ GeV, $p_T^{WW} < 30$ GeV

More good news on b physics

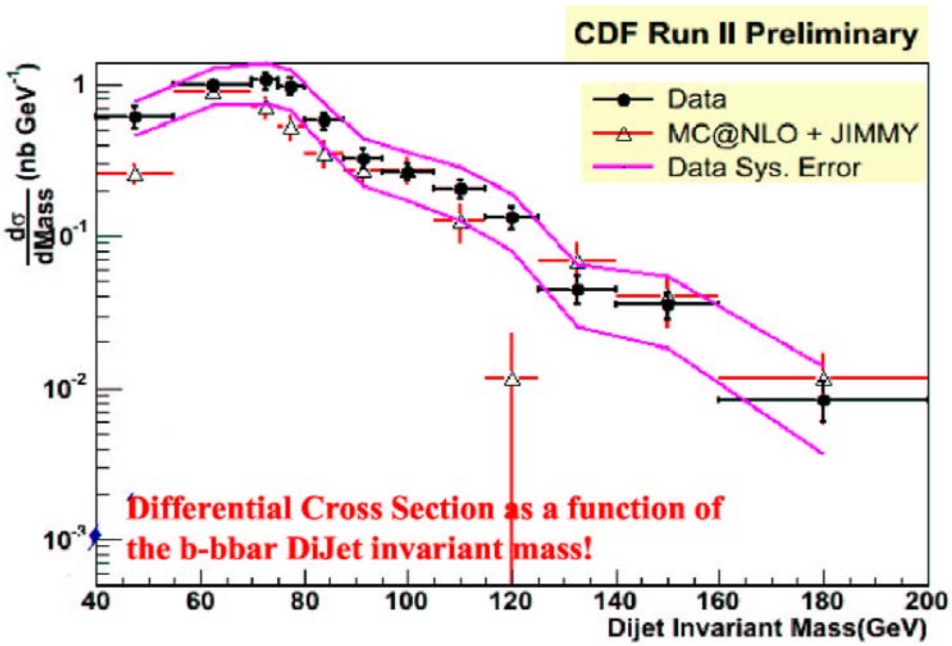


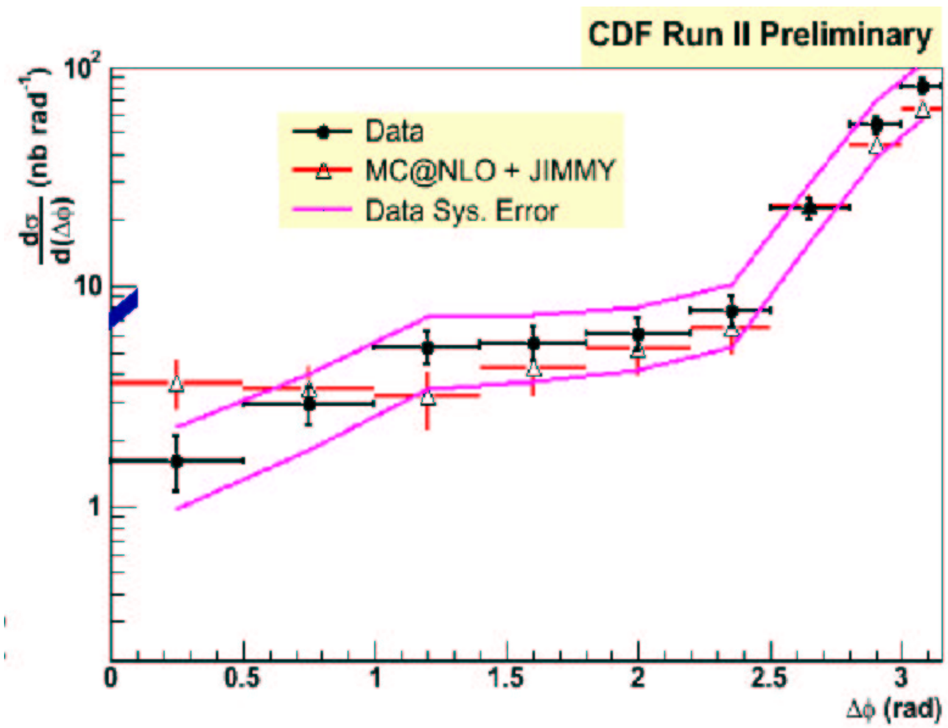


- These observables are very involved (b-jets at hadron level), and cannot be computed with analytic techniques
- The underlying event in Pythia is fitted to data; that of Herwig (used in MC@NLO) does not fit the data well (lack of MPI)

It's actually even better

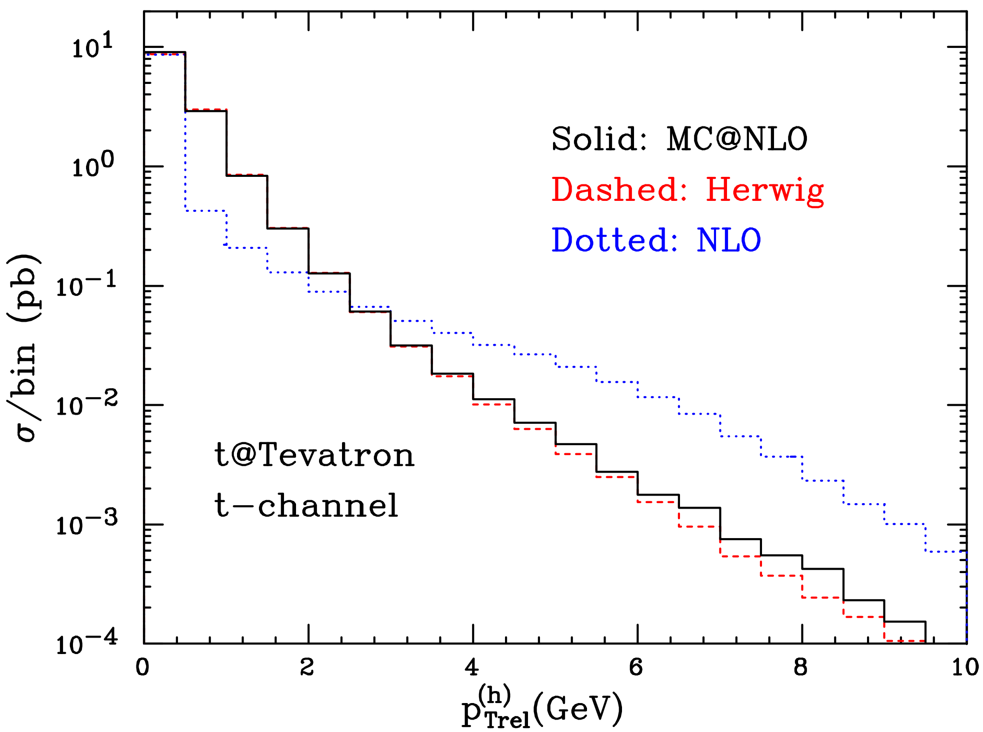
The treatment of the UE in Herwig recently improved: Jimmy

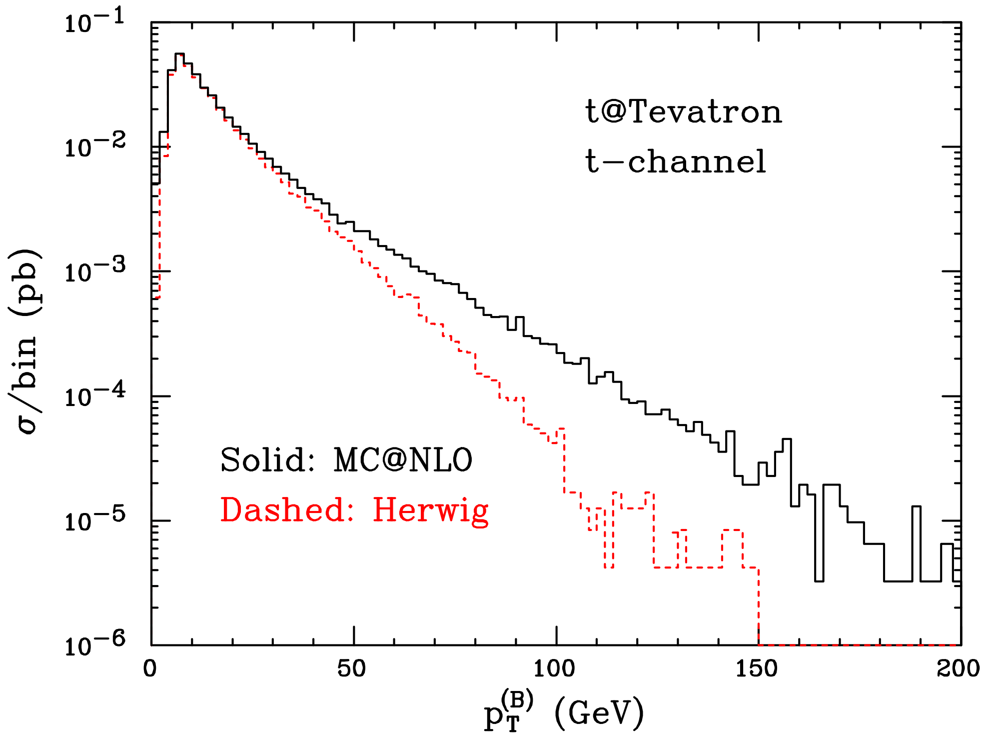




- The importance of the underlying event stresses the necessity of embedding a *precise* computation into a Monte Carlo framework, as done in MC@NLO

The ultimate test: single-top production





- Hadron p_T relative to the jet axis: hard emissions show up
- B-hadron p_T: hard emission effects are striking
  (but cannot be predicted by pure NLO)

There is ample evidence of MC@NLO improving both NLO computations and standard MC simulations

NLOwPS is a brand new field

Although somewhat undermanned, there is a lot of ongoing activity

- First working hadronic code: Φ-veto (Dobbs, 2001)
- Automated computations of ME's: grcNLO (GRACE group, 2003)
- Absence of negative weights (Nason, 2004)
- Showers with high log accuracy in ϕ_6^3 (Collins, Zu, 2002–2004)
- Proposals for $e^+e^- \to jets$ (Soper, Krämer, Nagy, 2003–2005; Giele, Kosower, 2006?)

The idea of including NLO matrix elements into MC's, however, dates back to the 80's. Why did it take so long to arrive at a working solution?

- The key point: the cancellation of IR singularities in an observable- and process-independent manner (sort of "exclusive"), as done in the universal subtraction formalisms

A similar understanding at NNLO would pave the way to NNLOwPS

Event generation in MC@NLO

- Compute the integrals

$$J_{\mathbb{H}} = \sum_{ab} \int dx_1\, dx_2\, d\phi_{n+1}\, f_a(x_1) f_b(x_2) \left| \mathcal{M}_{ab}^{(r)} - \mathcal{M}_{ab}^{(\mathrm{MC})} \right|$$

$$J_{\mathbb{S}} = \sum_{ab} \int dx_1\, dx_2\, d\phi_{n+1}\, f_a(x_1) f_b(x_2) \left| \mathcal{M}_{ab}^{(b,v,c)} - \mathcal{M}_{ab}^{(c.t.)} + \mathcal{M}_{ab}^{(\mathrm{MC})} \right|$$

- Get $N_{\mathbb{H}}$ $2 \to n+1$ events and $N_{\mathbb{S}}$ $2 \to n$ events, with

$$N_{\mathbb{H}} = N_{tot} \frac{J_{\mathbb{H}}}{J_{\mathbb{S}} + J_{\mathbb{H}}}\,, \qquad N_{\mathbb{S}} = N_{tot} \frac{J_{\mathbb{S}}}{J_{\mathbb{S}} + J_{\mathbb{H}}}$$

- For each phase-space point (x_1, x_2, ϕ_{n+1}), $\mathbb{H}$ and $\mathbb{S}$ kinematic configurations are unambiguously determined, and related by a map

$$\mathcal{P}_{\mathbb{H} \to \mathbb{S}}$$

An alternative event generation: βMC@NLO

- Compute the integral

$$J_{\mathbb{H}+\mathbb{S}} = \sum_{ab} \int dx_1\, dx_2\, d\phi_{n+1}\, f_a(x_1) f_b(x_2) \left| \mathcal{M}_{ab}^{(r)} + \mathcal{M}_{ab}^{(b,v,c)} - \mathcal{M}_{ab}^{(c.t.)} \right|$$

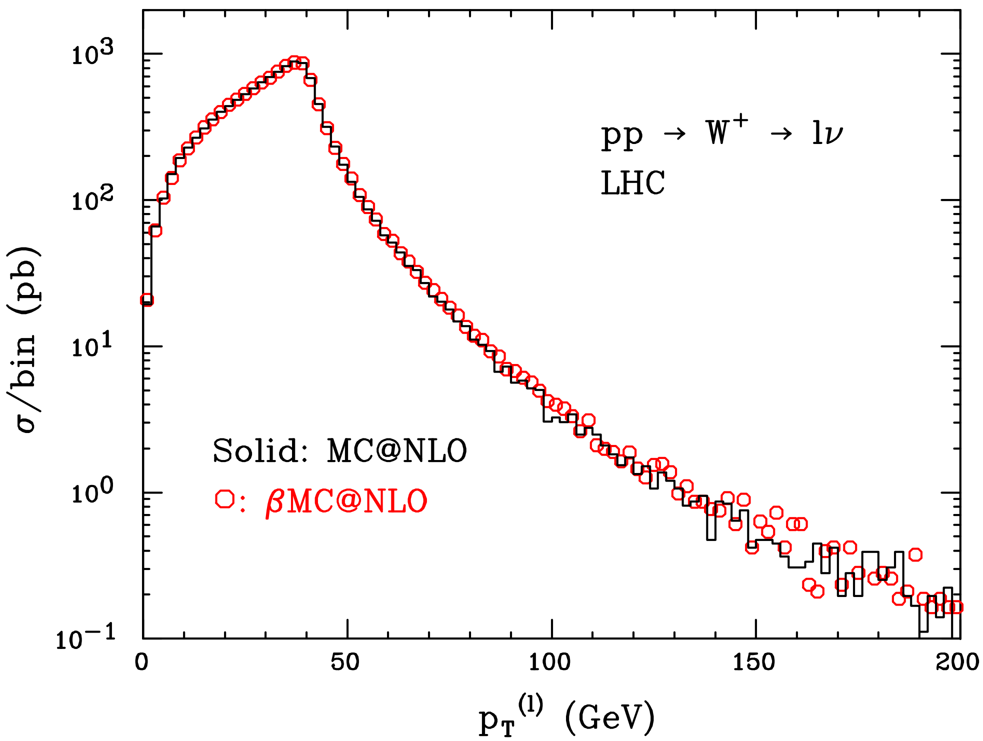
- For each phase-space point (x_1, x_2, ϕ_{n+1}), generate either $\mathbb{H}$ or $\mathbb{S}$ kinematics according to the ratio of weights

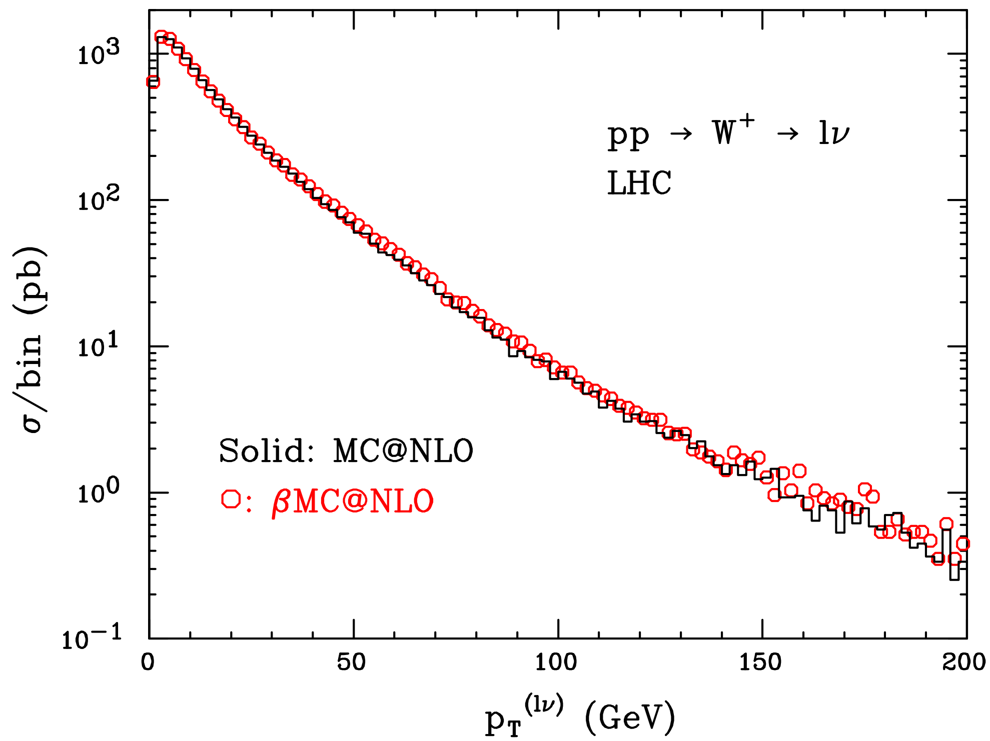
$$w_{\mathbb{H}} = \left| \mathcal{M}_{ab}^{(r)} - \mathcal{M}_{ab}^{(\mathrm{MC})} \right|, \qquad w_{\mathbb{S}} = \left| \mathcal{M}_{ab}^{(b,v,c)} - \mathcal{M}_{ab}^{(c.t.)} + \mathcal{M}_{ab}^{(\mathrm{MC})} \right|$$

- Tested in $e^+e^- \to$ 2 jets and $H_1 H_2 \to l\nu_l$: reduces the fraction of negative weights to less than 1%!

- But: expansion to $\mathcal{O}(\alpha_S \alpha_S^b)$ in the regions where the signs of $w_{\mathbb{H}}$ and $w_{\mathbb{S}}$ differ doesn't coincide with NLO $\longrightarrow$ double counting

$W^+ \longrightarrow l\nu_l$ with βMC@NLO





- No evidence of double counting in $e^+e^- \longrightarrow$ 2 jets and $H_1 H_2 \longrightarrow l\nu_l$
- Fractions of negative weights: 7.5%$\longrightarrow$ 0.03% (2 jets), 9%$\longrightarrow$ 0.8% ($l\nu_l$)

$w_{\mathbb{H}}$ and $w_{\mathbb{S}}$ have opposite signs only where $\mathcal{M}_{ab}^{(\text{MC})} \neq 0$
$\Longrightarrow$ NLO results are irrelevant there

βMC@NLO is a very interesting option, which is worth further studies

A step further

MC@NLO is based on a strategic assumption:

The Monte Carlo is a black box

- Advantage: the MC will not be modified, and will work as usual
- Disadvantage: a detailed knowledge of the MC is required

A different strategy: force the MC to "comply" with NLO

pMC@NLO (Nason (2004))

Basic idea: exponentiate *exact* real corrections into an MC Sudakov for the first emission

$$\widetilde{\Delta}(t_1, t_2) = \exp\left[-\alpha_S \int_{t_1}^{t_2} dt \frac{R}{tB}\right] \quad \longrightarrow \quad \widetilde{\mathcal{F}}_{\text{MC}}\left(\widetilde{\Delta}\Delta^n\right)$$

$$\mathcal{F}_{\text{pMC@NLO}} = \sigma_{tot}\widetilde{\mathcal{F}}_{\text{MC}}(0)\,, \qquad \sigma_{tot} = \text{total rate}$$

This is a simplified and somewhat imprecise notation

- Generate the hardest emission first, with $\widetilde{\Delta}(t_1, t_2)$
- Generate the remaining emissions with $\Delta(t_1, t_2)$ as usual

By generating the largest p_T in the first emission, angular ordering is violated

pMC@NLO vs MC@NLO

- All radiation through Sudakovs $\Longrightarrow$ no negative weights
- Largest p_T first $\Longrightarrow$ the MC must know how to handle *vetoed* showers
- The “right” ordering is in angle: need to introduce *vetoed & truncated* showers which restore colour coherence

Kinematics issues

MC@NLO: n-body matrix elements integrated over $(n+1)$-body phase space: definition of a projection $\mathcal{P}^{MC@NLO}_{\mathbb{H}\to\mathbb{S}}$

pMC@NLO: $(n+1)$-body matrix elements integrated at fixed variables for reduced n-body matrix elements: definition of a projection $\mathcal{P}^{pMC@NLO}_{\mathbb{S}\to\mathbb{H}}$

$\Longrightarrow$ *can* define $\mathcal{P}^{pMC@NLO}_{\mathbb{S}\to\mathbb{H}} = (\mathcal{P}^{MC@NLO}_{\mathbb{H}\to\mathbb{S}})^{-1}$

Outlook

MC@NLO "mainstream" (Del Duca, Laenen, Oh, Oleari, Motylinski, Webber, SF)

- Used for some $b\bar{b}$ and $t\bar{t}$ analysis at the Tevatron, and for several simulations at the LHC. MC's have increased their *predictive* power
- Increasing number of processes: currently working on dijets, spin corr in $t\bar{t}$ and single top, Wt mode for single top, Higgs in VBF

Theoretical developments

- New formalisms: MC@NLO is not an unique solution; pMC@NLO, which has no negative weights, is close to be formulated (Oleari, Nason, SF) in full generality. Work by several groups
- Inclusion of EW corrections into the formalism
- Automated one-loop computations into MC@NLO: increased flexibility
- General NNLO subtraction approaches $\longrightarrow$ NNLOwPS ?