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Parton Shower Monte Carlos: NLO QCD corrections

MCWS, Frascati, 27/2/2006

Memento

- In these days of “power showers”, we better keep in mind a simple fact: no matter what, 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

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

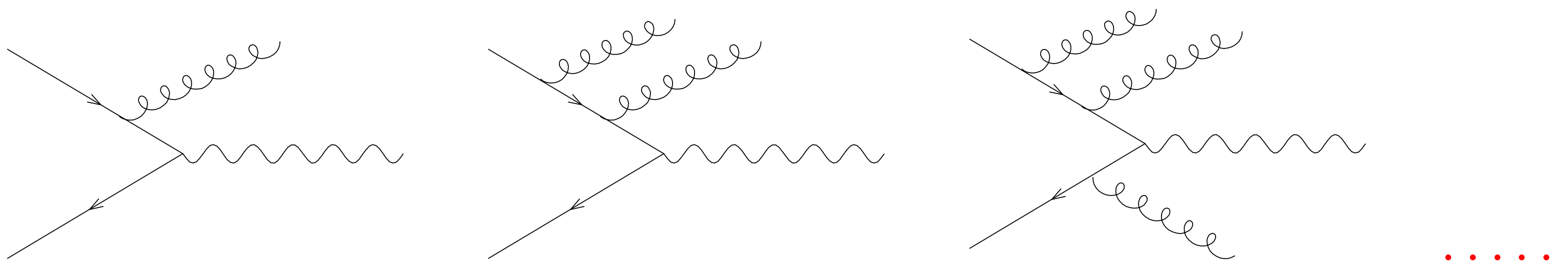
Which ones?

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

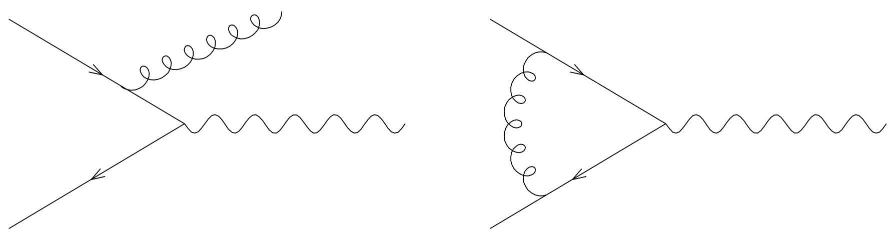
Solution

$\longrightarrow$ Catani's talk

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:

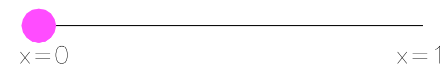
− The number of hard legs is smaller

− Computations are more complicated

NLO in a nutshell

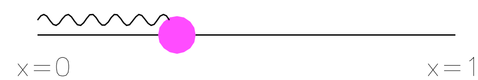
Think of the blob S as a $Q\overline{Q}$ pair in e^+e^- collisions. It radiates a gluon; all d.o.f. are integrated out, except the gluon energy. UV poles removed by renormalization

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



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

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



where $\lim_{x\to 0} R(x) = B$ (otherwise cross section diverges). An NLO prediction:

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

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

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

The computation of $d\sigma/dO$

Just compute (analytically, because of $1/\epsilon$) the integrals
$\longrightarrow$ won't work except for kinematically trivial observables

- Technically non-trivial, but otherwise a straightforward application of KLN theorem
- Fair enough if what you need is a single number (σ_{tot}, $g-2$, ...)

In the vast majority of the cases, the interest lies in the detailed knowledge of the final state: several differential cross sections with all sorts of kinematics cuts

The KLN theorem still holds bin-by-bin. But its implementation is a highly non-standard problem, which requires new ideas

The subtraction approach: real contribution

The real contribution has the most involved kinematics. Perform the following manipulation (Feynman?; Ellis, Ross, Terrano (1981))

$$\left(\frac{d\sigma}{dO}\right)_R = \alpha_S B\delta(O-O(0))\int_0^1 \frac{x^{-2\epsilon}}{x} + \alpha_S\int_0^1 dx\frac{R(x)\delta(O-O(x))-B\delta(O-O(0))}{x^{1+2\epsilon}}$$

that is, *add and subtract locally*

$$\alpha_S\frac{R(x)}{x}\delta(O-O(x)) \quad \xrightarrow{x\to 0} \quad \frac{\alpha_S B}{x}\delta(O-O(0))$$

The second integral is finite, thanks to the subtraction (of what is thus called counterterm)

$$\left(\frac{d\sigma}{dO}\right)_R = -\frac{\alpha_S B}{2\epsilon}\delta(O-O(0)) + \alpha_S\int_0^1 dx\frac{R(x)\delta(O-O(x))-B\delta(O-O(0))}{x}$$

- The *only* divergent term has now a B&V kinematics ⇒ cancellation independent of O

The subtraction approach: results

A non-trivial analytic integral has been replaced by a numerical integral

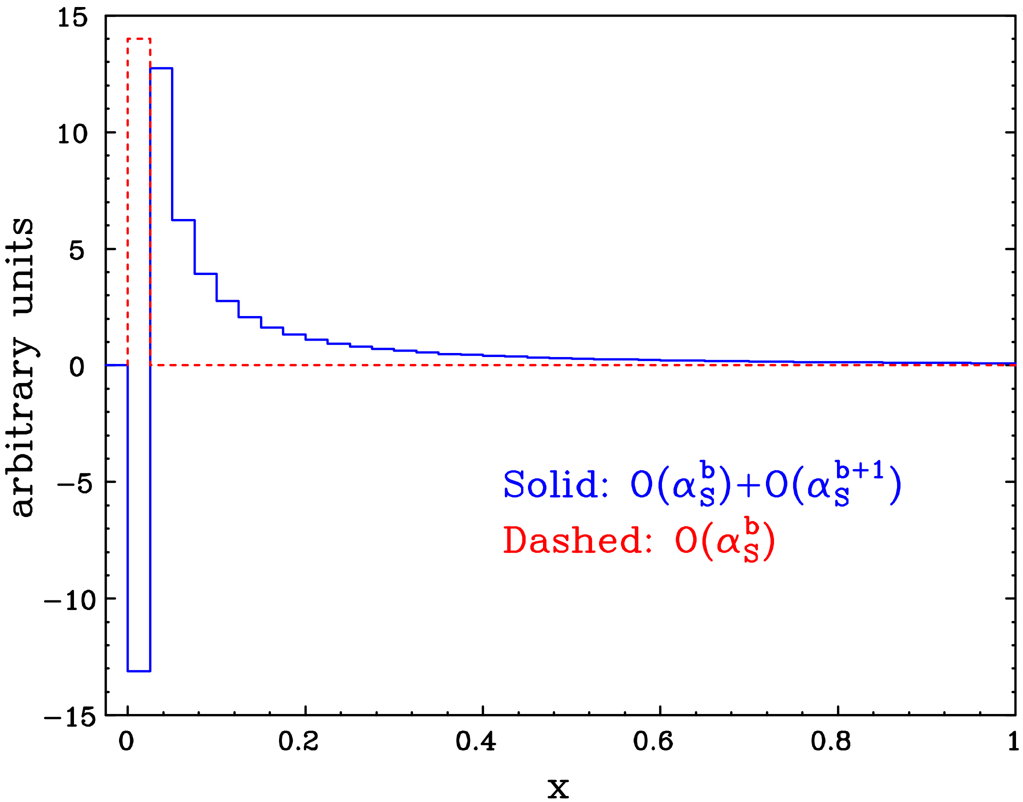
$$\left(\frac{d\sigma}{dO}\right)_{NLOsubt} = \int_0^1 dx \left\{ \delta(O - O(x)) \frac{\alpha_S R(x)}{x} \right.$$
$$\left. + \delta(O - O(0)) \left(B + \alpha_S V - \frac{\alpha_S B}{x} \right) \right\}$$

All of the (many) implementations of the method in the 80's and early 90's have been achieved starting from scratch. Later, it was realized that this is actually not necessary

$\longrightarrow$ Universal formalisms (see Oleari's talk)

How do the results look like?

Result for $O = x$



The positive and negative spikes will decrease upon increasing the bin size

QCD has finite resolution power

This does not look promising for exclusive observables: there are cancellations (*after* the removal of $1/\epsilon$ poles) between different final states

A toy LL MC

The system S 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 gluon be emitted with energy $x_1 < x < x_2$. The function $Q(z)$ parametrizes beyond-LL effects, with

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

The Born cross section

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

gives the overall normalization (B) and initial condition ((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)

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

Matching NLO with MC: NLOwPS

What do we want? Let's *define* it (SF, Webber (2002))

- 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

N^{n}LOwPS with $n \neq 1$ is unfeasible with our present understanding

NLO + MC $\longrightarrow$ NLOwPS?

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

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

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

It doesn't work:

- Cancellations between (x) and (0) 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))

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

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

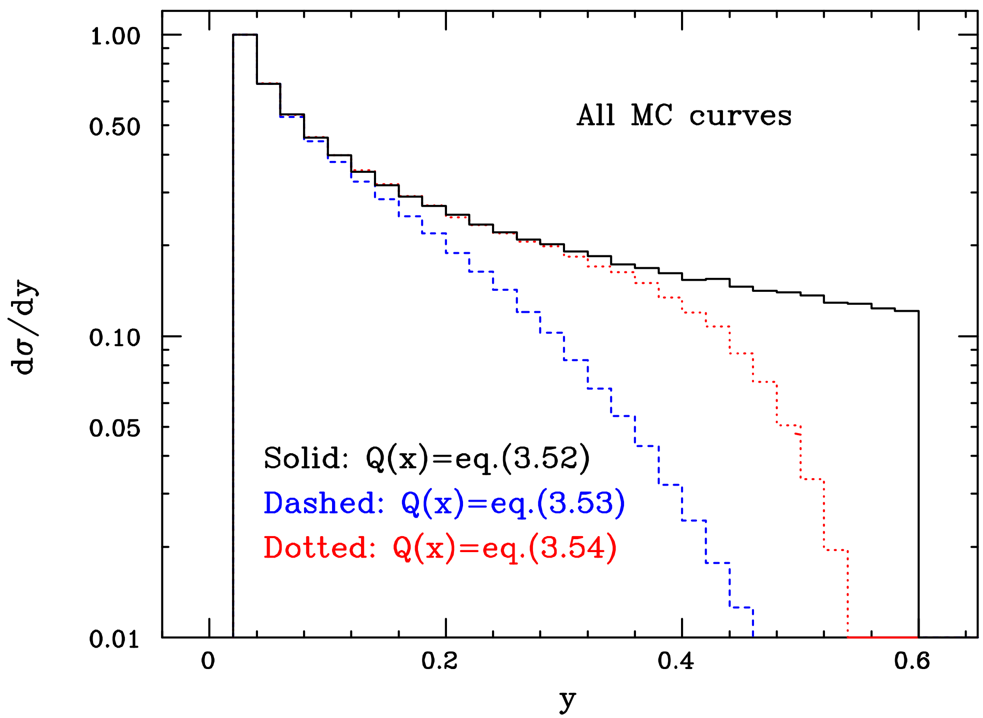
where the two (one for branching, one for no-branching probability) new terms are sensibly chosen:

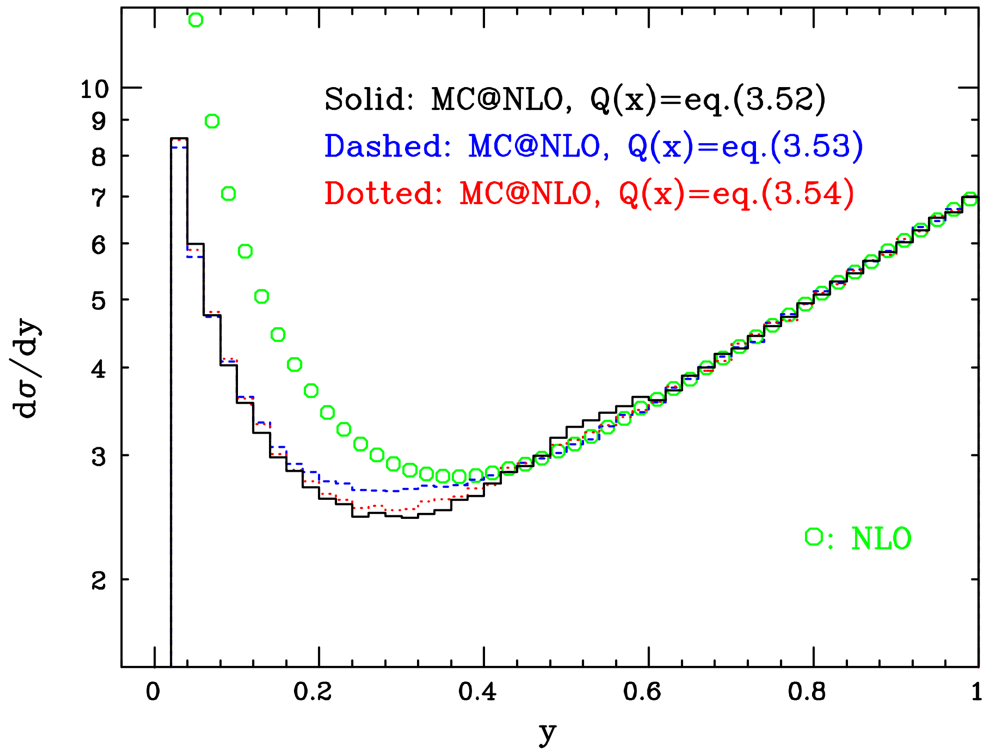
$$\left(\frac{d\sigma}{dx} \right)_{MC} = \alpha_S B \frac{Q(x)}{x} + \mathcal{O}(\alpha_S^2)$$

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

Toy model: results





1. $Q(x) = \Theta(x_{dead} - x);$
2. $Q(x) = \Theta(x_{dead} - x)G(x/x_{dead}),$ with $\alpha = 1, \beta = 1, c = 1;$
3. $Q(x) = \Theta(x_{dead} - x)G(x/x_{dead}),$ with $\alpha = 2, \beta = 1, c = 8.$

$$G(x) = \frac{c^2(1-x)^{2\beta}}{x^{2\alpha} + c^2(1-x)^{2\beta}}$$

- Very smooth transition across the dead zone border (good control beyond NLO)

MC@NLO: the QCD case

Strategy: follow what learned with the toy model

- Toy model

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

- QCD

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

Difficulties

As far as the modified subtraction is concerned, QCD is not that different from the toy model. There are however *at least* a couple of highly non-trivial issues

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

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

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

- The computation of the MC counterterms

$$\mathcal{M}_{ab}^{(\mathrm{MC})}(x_1, x_2, \phi_3)$$

requires a deep knowledge of MC implementation details. The *shower variables* have to be expressed in terms of the *phase-space variables* ϕ_3 used in the NLO computation

NLOwPS is a field in its infancy

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)

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

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: modify the MC

pMC@NLO (Nason (2004))

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

$$\widetilde{\Delta}(x_1, x_2) = \exp\left[-\alpha_S \int_{x_1}^{x_2} dz \frac{R(z)}{zB}\right] \quad \longrightarrow \quad \widetilde{\mathcal{F}}_{\rm MC}$$

$$\mathcal{F}_{\rm pMC@NLO} = \sigma_{tot} \widetilde{\mathcal{F}}_{\rm MC}(0)\,, \qquad \sigma_{tot} = B + \alpha_S V + \alpha_S \int_0^1 \frac{dx}{x}[R(x) - B]$$

This is a simplified and somewhat imprecise notation

Advantage: a detailed knowledge of the MC
is not required

Disadvantage: the MC will have to be modified

This is complementary to MC@NLO

pMC@NLO: QCD

The first emission sets an upper bound in p_T for the rest of the shower $\Longrightarrow$

- 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

It has been proved (Nason, 2004) that this is equivalent to moving the hardest emission up the shower: the first branching will be the hardest

- Negative weights basically gone
- May use a separate package for the vetoed & truncated showers
- Beyond-LL structure changed: need for re-tuning?
- |MC@NLO-pMC@NLO|$=\mathcal{O}(\alpha_S^2)$ $\longleftarrow$ how large α_S^2 terms?

Perspectives (for experimenters)

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

- 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

We now know how to do it. But we will do it only if the experimental community will show sufficient interest

- For the workshop: what are your priorities? Which processes?

Perspectives (for theorists)

A lot of interesting and rewarding work remains to be done

- This is theoretical physics proper, not code debugging*
- Much larger impact on phenomenology than any N^{k}LO results
- Dijets can now be done: a few months work for a young postdoc
- pMC@NLO has reached the implementation stage
- A lot of other improvements possible: large angles, beyond-LL, ...
- These techniques invented in QCD. How about QED?
- Obvious (and challenging) connections to automatization techniques
- NNLOwPS?

* OK, OK, just a tiny bit of that as well