Matching NLO QCD with Parton Showers

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- S Frixione & BRW, JHEP 0206(2002)029 [hep-ph/0204244]; hep-ph/0309186
- S Frixione, P Nason & BRW, JHEP $0308(2003)007~[\mathrm{hep-ph}/0305252]$
- V Del Duca, S Frixione, C Oleari & BRW, in preparation
- http://www.hep.phy.cam.ac.uk/theory/webber/MCatNLO/

Motivation

- Reliable prediction of cross sections and final-state distributions for QCD processes is important not only as a test of QCD but also for the design of collider experiments and new particle searches.
- All systematic approaches to this problem are based on perturbation theory, usually truncated at next-to-leading order (NLO).
- For the description of exclusive hadronic final states, perturbative calculations have to be combined with a model for the conversion of partonic final states into hadrons (hadronization). Existing hadronization models are in remarkably good agreement with a wide range of data, after tuning of model parameters.
- However, these models operate on partonic states with high multiplicity and low relative transverse momenta, which are obtained from a parton shower
 Monte Carlo (MC) approximation to QCD dynamics and not from fixed-order calculations.

Objectives

- Our aim is to develop a practical method for combining existing parton shower MC programs with NLO perturbative calculations (MC@NLO).
- We require MC@NLO to have the following characteristics:
 - ✤ The output is a set of events, which are fully exclusive.
 - ✤ Total rates are accurate to NLO.
 - ♦ NLO results for all observables are recovered upon expansion of MC@NLO results in α_s .
 - ♦ Hard emissions are treated as in NLO computations.
 - \clubsuit Soft/collinear emissions are treated as in MC.
 - \clubsuit The matching between hard- and soft-emission regions is smooth.
 - \clubsuit MC hadronization models are adopted.

Toy Model

- Consider first a toy model that allows simple discussion of key features of NLO, of MC, and of matching between the two.
 - ♦ Assume a system can radiate massless "photons", energy x, with $0 \le x \le x_s \le 1$, x_s being energy of system before radiation.
 - After radiation, energy of system is $x'_s = x_s x$.
 - System can undergo further emissions, but photons themselves cannot radiate.
- Task of predicting an infrared-safe observable *O* to NLO amounts to computing the quantity

$$\langle O \rangle = \lim_{\epsilon \to 0} \int_0^1 dx \, x^{-2\epsilon} O(x) \left[\left(\frac{d\sigma}{dx} \right)_{\rm B} + \left(\frac{d\sigma}{dx} \right)_{\rm V} + \left(\frac{d\sigma}{dx} \right)_{\rm R} \right]$$

where Born, virtual and real contributions are respectively

$$\left(\frac{d\sigma}{dx}\right)_{\rm \scriptscriptstyle B,V,R} = B\delta(x)\,, \quad a\left(\frac{B}{2\epsilon} + V\right)\delta(x)\,, \quad a\frac{R(x)}{x}\,,$$

a is coupling constant, and $\lim_{x\to 0} R(x) = B$.

• In subtraction method, real contribution is written as:

$$\langle O \rangle_{\rm R} = aBO(0) \int_0^1 dx \, \frac{x^{-2\epsilon}}{x} + a \int_0^1 dx \, \frac{O(x)R(x) - BO(0)}{x^{1+2\epsilon}} \, .$$

Second integral is non-singular, so we can set $\epsilon = 0$:

$$\left\langle O\right\rangle_{\mathrm{R}} = -a\frac{B}{2\epsilon}O(0) + a\int_{0}^{1}dx\,\frac{O(x)R(x) - BO(0)}{x}$$

• Therefore NLO prediction is:

$$\left\langle O\right\rangle_{\text{sub}} = BO(0) + a\left[VO(0) + \int_0^1 dx \,\frac{O(x)R(x) - BO(0)}{x}\right]$$

• We rewrite this in a slightly different form:

$$\langle O \rangle_{\text{sub}} = \int_0^1 dx \left[O(x) \frac{aR(x)}{x} + O(0) \left(B + aV - \frac{aB}{x} \right) \right]$$

Toy Monte Carlo

In a treatment based on Monte Carlo methods, the system can undergo an arbitrary number of emissions (branchings), with probability controlled by the Sudakov form factor, defined for our toy model as follows:

$$\Delta(x_1, x_2) = \exp\left[-a \int_{x_1}^{x_2} dz \frac{Q(x)}{x}\right]$$

where Q(x) is a monotonic function with the following properties:

$$0 \le Q(x) \le 1$$
, $\lim_{x \to 0} Q(x) = 1$, $\lim_{x \to 1} Q(x) = 0$

 $\Delta(x_1, x_2)$ is the probability that no photon be emitted with energy x such that $x_1 \leq x \leq x_2$.

Modified Subtraction

We want to interface NLO to MC. Naive first try:

 $O(0) \Rightarrow$ start MC with 0 real emissions: $\mathcal{F}_{MC}^{(0)}$ $O(x) \Rightarrow$ start MC with 1 emission at $x: \mathcal{F}_{MC}^{(1)}(x)$

so that overall generating functional is

$$\int_0^1 dx \left[\mathcal{F}_{\rm MC}^{(0)} \left(B + aV - \frac{aB}{x} \right) + \mathcal{F}_{\rm MC}^{(1)}(x) \frac{aR(x)}{x} \right]$$

• This is wrong: MC starting with no emissions will generate emission, with NLO distribution

$$\left(\frac{d\sigma}{dx}\right)_{\rm \scriptscriptstyle MC} = aB\frac{Q(x)}{x}$$

We must subtract this from second term, and add to first:

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

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

This prescription has several good features:

• $\mathcal{F}_{MC}^{(0)} = \mathcal{F}_{MC}^{(1)}$ to $\mathcal{O}(1)$, so added and subtracted terms are equal to $\mathcal{O}(a)$;

- Coefficients of $\mathcal{F}_{MC}^{(0)}$ and $\mathcal{F}_{MC}^{(1)}$ are now separately finite;
- Same resummation of large logs in $\mathcal{F}_{MC}^{(0)}$ and $\mathcal{F}_{MC}^{(1)} \Rightarrow \mathcal{F}_{MC@NLO}$ gives same resummation as $\mathcal{F}_{MC}^{(0)}$, renormalised to correct NLO cross section. Note, however, that some events may have negative weight.

Toy Model Observables

• As an example of an "exclusive" observable, we consider the energy y of the hardest photon in each event. The NLO and MC predictions are

$$\left(\frac{d\sigma}{dy}\right)_{\rm NLO} = a\frac{R(y)}{y}$$
$$\left(\frac{d\sigma}{dy}\right)_{\rm MC} = aB\frac{Q(y)}{y}\Delta(y,1)$$

As an "inclusive" observable, consider the fully inclusive distribution of photon energies, z:

$$\begin{pmatrix} \frac{d\sigma}{dz} \end{pmatrix}_{\text{NLO}} = a \frac{R(z)}{z} \\ \left(\frac{d\sigma}{dz} \right)_{\text{MC}} = a B \frac{Q(z)}{z}$$

• Toy model results below are for

$$a = 0.3, \quad B = 2, \quad V = 1,$$

 $R(x) = B + \frac{x}{9}(1 + \frac{x}{2} + 20x^2)$

For MC we have assumed a "dead zone" Q(x) = 0 for x > 0.6 with variable smoothing at boundary (see figure).



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Modified Subtraction for Real QCD

Consider a hadron collider process which is $2 \rightarrow 2$ at LO, e.g. W⁺W⁻ or $Q\bar{Q}$ pair production. Schematic expression for any observable O, evaluated by subtraction method, is

$$\langle O \rangle_{\text{sub}} = \sum_{ab} \int_0^1 dx_1 \, dx_2 \, d\phi_3 \, f_a(x_1) f_b(x_2) \left[O^{(2 \to 3)} \mathcal{M}_{ab}^{(h)}(x_1, x_2, \phi_3) \right. \\ \left. + O^{(2 \to 2)} \left(\mathcal{M}_{ab}^{(b,v,c)}(x_1, x_2, \phi_2) - \mathcal{M}_{ab}^{(c.t.)}(x_1, x_2, \phi_3) \right) \right]$$

- ★ M^(h)_{ab} is NLO real-emission contribution;
 ★ M^(b,v,c)_{ab} are LO Born, NLO virtual and collinear (finite parts);
 ★ M^(c.t.)_{ab} are counter-terms which cancel divergences of M^(h)_{ab}.
- Naively, for MC@NLO we would replace $O^{(2\to 2,3)}$ by $\mathcal{F}_{MC}^{(2\to 2,3)}$ (MC generating functionals starting from $2\to 2, 3$ hard subprocesses), to obtain $\mathcal{F}_{MC@NLO}$.
- This would be wrong because $\mathcal{F}_{MC}^{(2\to2)}$ also generates $2 \to 3$ configurations, which must be subtracted from weight of $\mathcal{F}_{MC}^{(2\to3)}$ (and added to that of $\mathcal{F}_{MC}^{(2\to2)}$).

• Therefore for MC@NLO we define

$$\begin{aligned} \mathcal{F}_{\rm MC@NLO} &= \sum_{ab} \int_0^1 dx_1 \, dx_2 \, d\phi_3 \, f_a(x_1) f_b(x_2) \\ & \left[\mathcal{F}_{\rm MC}^{(2 \to 3)} \left(\mathcal{M}_{ab}^{(h)}(x_1, x_2, \phi_3) - \mathcal{M}_{ab}^{(\rm MC)}(x_1, x_2, \phi_3) \right) + \right. \\ & \left. \mathcal{F}_{\rm MC}^{(2 \to 2)} \left(\mathcal{M}_{ab}^{(b,v,c)}(x_1, x_2, \phi_2) - \mathcal{M}_{ab}^{(c.t.)}(x_1, x_2, \phi_3) + \mathcal{M}_{ab}^{(\rm MC)}(x_1, x_2, \phi_3) \right) \right] \end{aligned}$$

- Provided MC does a good job in all soft and collinear limits, coefficients of $\mathcal{F}_{MC}^{(2\to2)}$ and $\mathcal{F}_{MC}^{(2\to3)}$ are now separately finite.
- But coefficients may be negative \Rightarrow some events have negative weight.
- Number of negative weights can be reduced by tuning counterterms. Typically we find 10 20%.

W^+W^- Observables



These correlations are problematic: the soft and hard emissions are both relevant. MC@NLO does well, resumming large logarithms, and yet handling the large-scale physics correctly

Solid: MC@NLO Dashed: HERWIG $\times \frac{\sigma_{NLO}}{\sigma_{LO}}$ Dotted: NLO

Jet Observables in W^+W^- Production



Jets have been reconstructed with a k_T algorithm. It is striking that inclusive jet distribution displays the same behaviour as in the toy model: MC@NLO/MC=K factor for $p_T \rightarrow 0$

Solid: MC@NLO Dashed: HERWIG $\times \frac{\sigma_{NLO}}{\sigma_{LO}}$

W^+Z Observables



It is interesting that the MC@NLO fills further the kinematic dip at $\eta_{W^+} - \eta_Z = 0$. The difference between MC@NLO and MC is enhanced by the cuts in the $\Delta \phi$ tail

Solid: MC@NLO Dashed: HERWIG $\times \frac{\sigma_{NLO}}{\sigma_{LO}}$ Dotted: NLO

Heavy Quark Production

- Modified subtraction formula above can be used for any process.
 - \clubsuit Take standard subtraction formula;
 - ✤ Calculate analytically exactly what MC does at NLO;
 - Insert $\mathcal{M}_{ab}^{(\mathrm{MC})}(x_1, x_2, \phi_3)$ terms;
 - ♦ Generate $2 \rightarrow 2$ and $2 \rightarrow 3$ parton configurations and weights;
 - \clubsuit Feed into MC (using Les Houches interface, hep-ph/0109068).
- Most difficult part is calculating what MC does!
 - ✤ Details in FNW, JHEP 0308(2003)007 [hep-ph/0305252]

MC Heavy Quark Production

• MC starts from $2 \rightarrow 2$ subprocess \Rightarrow momentum reshuffling is done after real emission.



- Relation between invariants and shower variables depends on which leg emits!
- Colour structure assigned (for shower/hadronization) according to $N \to \infty$ limit.



t, \bar{t} Observables at Colliders





Solid: MC@NLO Dashed: HERWIG $\times \frac{\sigma_{NLO}}{\sigma_{LO}}$ Dotted: NLO MC@NLO \simeq NLO here. New feature in MC: $Q\overline{Q}$ asymmetry at Tevatron.

Top Rapidity Asymmetry at Tevatron



$t\bar{t}$ Correlations at LHC



These correlations display the same patterns as those for vector boson pair production. Hard- and soft-scale physics are both treated correctly.

Solid: MC@NLO Dashed: HERWIG $\times \frac{\sigma_{NLO}}{\sigma_{LO}}$ Dotted: NLO

$b\overline{b}$ Correlations at Tevatron



HERWIG does well (after cuts) but needs much more CPU: 14 million events vs 1 million for MC@NLO Solid: MC@NLO Dashed: HERWIG (no K-factor) Dotted: NLO

b Production with HERWIG

• In parton shower MC's, 3 classes of processes can contribute:



All are needed to get close to data (RD Field, hep-ph/0201112):



GSP and FEX contributions in HERWIG



• GSP, FEX and FCR are complementary and all must be generated

- \clubsuit GSP cutoff (PTMIN) sensitivity depends on cuts and observable
- \clubsuit FEX sensitive to bottom PDF
- ♦ GSP efficiency very poor, $\sim 10^{-4}$
- All these problems are avoided with MC@NLO!

$NLO + k_T$ -kick vs MC@NLO

• (NLO + k_T -kick) with $\langle k_T \rangle = 4 \text{ GeV} \simeq \text{MC@NLO}$ (at Tevatron)



• This does NOT mean that there is $\langle k_T \rangle = 4$ GeV inside proton: it simply emulates the effect of initial-state parton showers.

Hadron-level Results on B production

• $B \rightarrow J/\psi$ results from Tevatron Run II \Rightarrow B hadrons (includes BR's)



• No significant discrepancy!

Associated Higgs + Vector Boson Production

• Associated Higgs production implemented with full decay correlations



• LO in HERWIG 6.506, NLO in MC@NLO 3.1 (in preparation)

Associated Higgs + Vector Boson Production

• p_t of WH pair in $\bar{p}p \to W^+H^0X$ at Tev II



• Qualitatively similar to WW

Associated Higgs + Vector Boson Production (cont'd)

• WH azimuthal separation in $\bar{p}p \to W^+ H^0 X$ at Tev II



Unassociated Higgs Production at LHC

• Good agreement with (N)NLO+NNLL



Conclusions and Future Prospects

- MC@NLO exists and works well for W, Z, H, WW, WZ, ZZ, WH, ZH, $t\bar{t}$ and $b\bar{b}$ production. Negative weights ~ 10% ($t\bar{t}$) to 20% ($b\bar{b}$) not a problem.
- Decay correlations implemented for W, Z, WH, ZH, not yet for others.
- Jet production needs more work.
- Shower modification to avoid negative weights looks possible (P Nason).
- General interface to NLO (subtraction method) programs feasible.