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# Shower Monte Carlo's at Next-to-Leading Order: POWHEG

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LoopFest 2009, Madison, May 7th 2009

# Outline

Introduction:

• Motivations for NLO+Shower

Understanding differences:

- Formal comparison of POWHEG and MC@NLO
- Comparison of phenomenological results

Complex processes and automation:

- POWHEG for complex processes: flavour and singularities separation
- Full automation in POWHEG: the POWHEG BOX
- Conclusions

#### Why NLO+Shower

- NLO results are cumbersome to use; they yield differential cross sections that are not positive definite (that in fact have canceling positive and negative infinities).
- Experimental results can be compared to NLO results only after unfolding detector effects. With NLO+Showers one can feed the output through detector simulation, and compare to raw data.
- Experimentalists have always asked for it (and sometimes tried hard to do it themselves).
- It can be done: it should be done!

Two methods developed at the level of producing usable implementations for collider physics: MC@NLO and POWHEG.

Alternative proposals: Kramer, Mrenna, Soper  $(e^+e^- \rightarrow 3 \text{ partons})$ , MC@NLO variants based upon alternative shower algorithms:

- Shower by antenna factorization (Frederix, Giele, Kosower, Skands) (toy implementation for  $H \rightarrow gg$ )
- Shower by Catani-Seymour dipole factorization (Schumann)
- Shower with quantum interference (Nagy, Soper)
- Shower by Soft Collinear Effective Theory (Bauer, Schwartz)

#### MC@NLO (2002, Frixione+Webber)



Add difference between exact NLO and approximate (MC) NLO.

- Must use MC kinematics
- Difference should be regular (if the MC is OK)
- Difference may be negative

Several collider processes already there: Vector Bosons, Vector Bosons pairs, Higgs, Single Top (also with W), Heavy Quarks, Higgs+W/Z.

### POWHEG

#### Positive Weight Hardest Emission Generator

Method to generate the hardest emission first, with NLO accuracy, and independently of the SMC (P.N. 2004).

- SMC independent; no need of SMC expert; same calculation can be interfaced to several SMC programs with no extra effort
- SMC inaccuracies in the soft region only affect next-to-hardest emissions; no matching problems
- As the name says, it generates events with positive weight

### Status of POWHEG

Up to now, the following processes have been implemented in POWHEG:

- $hh \rightarrow ZZ$  (Ridolfi, P.N., 2006)
- $e^+e^- \rightarrow \text{hadrons}$ , (Latunde-Dada, Gieseke, Webber, 2006),  $e^+e^- \rightarrow t\bar{t}$ , including top decays at NLO (Latunde-Dada, 2008),
- $hh \rightarrow Q\bar{Q}$  (Frixione, Ridolfi, P.N., 2007)
- $hh \rightarrow Z/W$  (Alioli, Oleari, Re, P.N., 2008; ) (Hamilton, Richardson, Tully, 2008;)
- $hh \rightarrow H$  (gluon fusion) (Alioli, Oleari, Re, P.N., 2008; Herwig++)
- $hh \rightarrow H$ ,  $hh \rightarrow HZ/W$  NEW (Hamilton, Richardson, Tully, 2009;)
- $hh \rightarrow t + X$  (single top) NEW (Alioli, Oleari, Re, P.N., 2009)
- $hh \rightarrow Z + jet$ , Very preliminary (Alioli, Oleari, Re, P.N., 2009)
- The POWHEG BOX, Very preliminary, (Alioli, Oleari, Re, P.N., 2009)

### Formal comparison of POWHEG and MC@NLO

From now on:

- Assume that only one line radiates
- $\Phi_B$  is the phase space of the Born level process
- $\Phi$  is the phase space of the real matrix elements
- Assume a factorization  $d\Phi = d\Phi_B d\Phi_r$ , with  $d\Phi_r$  is 3-dimensional
- $B(\Phi_B)$  is the Born cross section
- $R(\Phi_B, \Phi_r) = R(\Phi)$  is the real cross section

MC@NLO and POWHEG implement the Hardest emission according to the formula

$$d\sigma = d\Phi_{\scriptscriptstyle B}\bar{B}(\Phi_{\scriptscriptstyle B}) \Big[ \Delta_{t_0} + \Delta_t \frac{R_s(\Phi)}{B(\Phi_{\scriptscriptstyle B})} d\Phi_r \Big] + R_f d\Phi, \quad \Delta_t = \exp \Big[ -\int \frac{R_s}{B} d\Phi_r \,\theta(k_T - t) \Big]$$

In standard SMC:  $\bar{B} = B$ ,  $R_s = R^{\text{MC}} = B \frac{\alpha_s(t)}{2\pi} \frac{P_{i,jk}(z)}{t}$ ,  $R_f = 0$ ,  $d\Phi_r = d\Phi_r^{\text{MC}} = dt dz d\phi$ 

In MC@NLO: 
$$\bar{B}^{MC}(\Phi_B) = B(\Phi_B) + \underbrace{\left[\underbrace{V(\Phi_B)}_{\text{infinite}} + \underbrace{\int R^{MC}(\Phi_B, \Phi_r^{MC}) d\Phi_r^{MC}}_{\text{infinite}}\right]}_{\text{finite}},$$

$$R_s = R^{\text{MC}}, \qquad R_f = R - R^{\text{MC}}, \qquad d\Phi_r = d\Phi_r^{\text{MC}}$$

MC@NLO generates  $\Phi_B$  distributed according to  $\bar{B}^{MC}$  (the hardest radiation is generated by the MC shower machinary) and  $\Phi$  according to  $R_f$ .

In POWHEG: 
$$\bar{B}(\Phi_B) = B(\Phi_B) + \underbrace{\bigcup_{\text{infinite}} V(\Phi_B) + \underbrace{\bigcup_{\text{infinite}} R_s(\Phi_B, \Phi_r) d\Phi_r}_{\text{infinite}}}_{\text{finite}}, \quad R_s + R_f = R_s$$

 $R_f$  must be regular and positive. Normally:  $R_f = 0, R_s = R$ .

Radiation is generated by POWHEG. Subsequent, less hard radiation is provided by the SMC to which POWHEG is interfaced

Accuracy: 
$$d\sigma = d\Phi_B \bar{B}(\Phi_B) \Big[ \Delta_{t_0} + \Delta_t \frac{R_s(\Phi)}{B(\Phi_B)} d\Phi_r \Big] + R_f d\Phi$$

Small 
$$k_T$$
:  $\frac{R_s(\Phi)}{B(\Phi_B)} d\Phi_{rad} \approx \frac{\alpha_s(t)}{2\pi} P_{i,jk}(z) \frac{dt}{t} dz \frac{d\phi}{2\pi}$ ,  
Also:  $\bar{B} \approx B \times (1 + \mathcal{O}(\alpha_s))$ 

Thus: all features of SMC's are preserved at small  $k_T$ .

Large  $k_T$ :  $\Delta \to 1$ ,  $d\sigma = \bar{B} \times \frac{R_s}{B} d\Phi + R_f d\Phi \approx R_s \times (1 + \mathcal{O}(\alpha_s)) d\Phi + R_f d\Phi$ ,

so: large  $k_t$  accuracy is preserved.

**NLO** accuracy: since  $\Delta_{t_0} + \int \Delta_t \frac{R_s(\Phi)}{B(\Phi_B)} d\Phi_r = 1$ , integrating in  $d\Phi_r$  at fixed  $\Phi_B$ 

$$\int \! \delta (\Phi_{\scriptscriptstyle B} - \bar{\Phi}_{\scriptscriptstyle B}) \, d\sigma = \left[ \bar{B} + \int \! R_f \, d\Phi_r \right]_{\Phi_{\scriptscriptstyle B} = \bar{\Phi}_{\scriptscriptstyle B}} = \left[ B + V + \int \left( R_s + R_f \right) d\Phi_r \right]_{\Phi_{\scriptscriptstyle B} = \bar{\Phi}_{\scriptscriptstyle B}}$$

So: NLO accuracy is preserved for inclusive quantities.

Although MC@NLO and POWHEG yield the exact NLO cross section, differential distributions are affected by induced NNLO terms:

$$d\sigma = d\Phi_{\scriptscriptstyle B}\bar{B}\Big[\Delta_{t_0} + \Delta_t \frac{R_s}{B} d\Phi_r\Big] + R_f d\Phi, \qquad R_s + R_f = R, \qquad \bar{B} = B + \left[V + \int R_s \, d\Phi_r\right]$$

The expression for  $\Delta_{t_1,t} = \exp\left[-\int \frac{R}{B} d\Phi_r \theta(k_T - t)\right]$  generates terms of all orders, and suppresses the distributions at small  $p_T$ .

The square bracket term in  $\overline{B}$ , multiplied by  $R_s/B$ , generates NNLO terms (in case of positive NLO corrections, it typically enhances the distributions.)

## POWHEG: Interfacing to SMC's

POWHEG is completely detached from the SMC to which it is interfaced. It uses the standard Les Houches Interface for User's Processes (LHI):

The LHI provides a facility to pass the  $p_T$  of the event to the SMC, so that no radiation harder than  $p_T$  will be generated by the MC.

For angular ordered showers (i.e. HERWIG), to preserve double log accuracy one should provide truncated showers (P.N. 2004), now implemented in HERWIG++.

## Examples: Z production

HERWIG alone fails at large  $p_T$ ; NLO alone fails at small  $p_T$ ; MC@NLO and POWHEG work in both regions;

#### Notice:

HERWIG with ME corrections or any ME program, give the same NLO shape at large  $p_T$ However: Normalization around small  $p_T$  region is incorrect (i.e. only LO).



# Comparisons of POWHEG+HERWIG vs. MC@NLO

### Z pair production







Remarkable agreement for most quantities;

### POWHEG and MC@NLO comparison: Top pair production



Good agreement for most observables considered (differences can be ascribed to different treatment of higher order terms)

#### Bottom pair production



- Very good agreement For large scales (ZZ,  $t\bar{t}$  production)
- Differences at small scales ( $b\bar{b}$  at the Tevatron)
- POWHEG more reliable in extreme cases like  $b\bar{b}, c\bar{c}$  at LHC (yields positive results, MC@NLO has problems with negative weights)

### Z production: POWHEG+HERWIG vs. MC@NLO



Small differences in high and low  $p_T$  region

## Z production: rapidity of hardest jet (TEVATRON)



### Dip in central region in MC@NLO also in $t\bar{t}$ and ZZ



### ALPGEN and $t\bar{t} + jet$ at NLO vs. MC@NLO



POWHEG distribution as in ALPGEN (Mangano, Moretti, Piccinini, Treccani, Nov.06) and in  $t\bar{t} + jet$  at NLO (Dittmaier, Uwer, Weinzierl) : no dip present.

# Higgs boson via gluon fusion at LHC



## Jet rapidity in h production



Dip in MC@NLO inerithed from even deeper dip in HERWIG (MC@NLO tries to fill dead regions in HERWIG, a mismatch remains).

Gets worse for larger  $E_T$  cuts:



#### Questions:

Why MC@NLO has a dip in the hardest jet rapidity?

Why POWHEG has no dip? Is that because of the hardest  $p_T$  spectrum?

Hard  $p_T$  spectrum in POWHEG POWHEG vs. NNLO vs. NNLL



Large enhancement because of the large K factor in Higgs production. Better agreement with NNLO this way. There is enough flexibility in POWHEG to get rid of it (if one wants)!!!

In the POWHEG cross section:

$$d\sigma' = d\Phi_{\scriptscriptstyle B} \bar{B}^{s} \left[ \Delta^{s}_{t_{0}} + \Delta^{s}_{t} \frac{R_{s}}{B} d\Phi_{r} \right] + R_{f} d\Phi$$

with:

$$\Delta_t^s = \exp\left[-\int \theta(t_r - t) \frac{R_s}{B} d\Phi_r\right].$$

Rather than choosing  $R_f = 0, R_s = R$ , choose

$$R_f = R \frac{k_T^2}{k_T^2 + h^2}, \quad R_f = R \frac{h^2}{k_T^2 + h^2};$$





No new features (dips and the like) arise in the other distributions:



So: high  $k_T$  cross section and dips are unrelated issues.

#### Why is there a dip in MC@NLO?

$$d\sigma = \underbrace{d\Phi_{B}\bar{B}^{MC}}_{S \text{ event}} \left[ \underbrace{\Delta_{t_{0}}^{MC} + \Delta_{t}^{MC} \frac{R^{MC}}{B} d\Phi_{r}^{MC}}_{\text{HERWIG shower}} \right] + \left[ \underbrace{R - R^{MC}}_{H \text{ event}} \right] d\Phi$$
$$\bar{B}^{MC} = B + \left[ V + \int R^{MC} (\Phi_{B}, \Phi_{r}) \, d\Phi_{r} \right]$$

For large  $k_T$ :

$$d\sigma = \frac{\bar{B}^{\rm MC}}{B} R^{\rm MC} d\Phi_{\rm B} d\Phi_{\rm r}^{\rm MC} + [R - R^{\rm MC}] d\Phi$$

$$=\underbrace{Rd\Phi}_{\text{nodip}} + \underbrace{\left(\frac{B^{\text{HW}}}{B} - 1\right)}_{\mathcal{O}(\alpha_s), \text{ but large for Higgs}} \times \underbrace{R^{\text{HW}}_{\text{Pure Herwig dip}} d\Phi$$

So: a contribution with a dip is added to the exact NLO result; The contribution is  $\mathcal{O}(\alpha_s R)$ , i.e. NNLO!

Can we test this hypothesis? Replace  $\bar{B}^{HW}(\Phi_n) \Rightarrow B(\Phi_n)$  in MC@NLO! the dip should disappear ...

#### MC@NLO with $B^{HW}$ replaced by B



No visible dip is present! (on the right track ...)

#### Detailed study of the problem also by Hamilton, Richardson, Tully, 2009



Both HERWIG and HERWIG++ have a dead radiation region corresponding to central rapidity and high energy. Dip in central region in HERWIG can be attributed to the dead zone.



#### Summary of MC@NLO and POWHEG comparisons

- Fairly good agreement on most distributions
- Areas of disagreement can be tracked back to NNLO terms, arising mostly because of the use of an NLO inclusive cross section (the B
  function) to shower out the hardest radiation.
- In POWEG, since the hardest radiation is generated by POWHEG itself, one has high flexibility in tuning the magnitude of these NNLO terms.
- For MC@NLO, these NNLO terms can generate unphysical behaviour in physical distributions, reflecting the dead zones structure of the underlying shower Monte Carlo. Since MC@NLO uses the underlying MC to generate the hardest emission, it is difficult to remedy to these problems without intervening on the MC itself

#### Flavour and singularities separation

The separation of the different singular regions is based upon the general formulation of POWHEG given in Frixione, Oleari, P.N. 2007.

There are several allowed flavour assignments in the n body process. B and V contributions are labelled by the flavour structure index  $f_b$ .

There are several allowed flavour structures in the n+1 body process. Thus R is labelled by a flavour structure index  $f_r$ . Each component  $R_{f_r}$  has several singularity regions. We thus write

$$R = \sum_{\alpha_r} R^{\alpha_r}$$

where each  $R^{\alpha_r}$  has a specific flavour structure, and is singular in only one singular region. In FKS one writes

$$R^{\alpha_r} = R_{f_r} \times \mathcal{S}_{\alpha_r}, \qquad \sum_{\alpha_r} S_{\alpha_r} = 1$$

The  ${\cal S}$  factors in the FKS formalism are defined as

$$S_i = \frac{1}{Nd_i}, \ S_{ij} = \frac{1}{Nd_{ij}} h\left(\frac{E_i}{E_i + E_j}\right),$$

where N is define so that  $\sum_{\alpha_r} S_{\alpha_r} \!=\! 1$  ,

$$d_i = \left(\sqrt{s}E_i/2\right)^a (1 - \cos^2\theta_i)^b, \quad d_{ij} = (E_iE_j)^a (1 - \cos\theta_{ij})^b,$$
$$\lim_{z \to 0} h(z) = 1, \quad \lim_{z \to 1} h(z) = 0, \quad h(z) + h(1 - z) = 1.$$

For example:

$$h(z) = \frac{(1-z)^c}{z^c + (1-z)^c}$$

So, the  $S_i$  factors single out the region where parton i is collinear to either initial state line, or is soft, while  $S_{ij}$  single out the region where parton i is collinear to parton j or is soft.

### The underlying Born

This is a basic concept in the POWHEG formalism; To each region  $\alpha_r$  we associate an underlying Born flavour configuration  $f_b$ , obtained as follows:

- If the singular region is associated to a parton becoming soft, then the parton must be a gluon, and it is simply removed to get the underlying Born configuration
- If the region is associated to two parton becoming collinear, then, in order for the region to be singular, the two partons must come from the splitting of another parton. The two partons are removed, and are replaced by the single parent parton with the appropriate flavour

Notice that in a shower Monte Carlo one first generates the Born process (i.e. the underlying Born configuration) and then lets one initial or final line undergo collinear splitting. Here we look at each singular region of the real matrix element, and ask from which underlyng Born process it could have been produced via a shower.

#### The underlying Born kinematics

To each kinematic configuration for the full radiation phase space  $\Phi$ , one associates an underlying Born kinematics  $\Phi_B$  and a set of radiation variables  $\Phi_r = (y, z, \phi)$ . For initial state radiation  $\Phi_B$  is obtained by going with a longitudinal boost to the frame where the system recoiling against radiation has zero longitudinal momentum. In this frame one boosts the recoil system in the transverse direction, so that its transverse momentum becomes zero



The radiation variables are  $y = \cos \theta$ ,  $\theta$  being the angle between the radiated parton and the positive rapidity incoming parton,  $\xi = 2E/\sqrt{s}$ , where E is the energy of the radiated parton, and  $\phi$  is its azimuth.

For final state radiation, the splitting partons are merged by summing their 3-momenta in the partonic CM frame. The 3-momentum is scaled, and the recoil system is boosted so that momentum and energy are conserved.



The radiation variables are  $y = \cos \theta$ ,  $\theta$  being the angle between the radiated partons,  $\xi = 2E_i/\sqrt{s}$ ,  $\phi$  is the azimuth of the ij plane relative to  $\vec{k_i} + \vec{k_j}$ . (This differs from FKS kinematics , where  $\phi$  is relative to  $\vec{k_j}$ ). The  $\overline{B}$  function carries a flavour structure index, and is given by

$$\bar{B}^{f_b}(\Phi_B) = \left[B(\Phi_B) + V(\Phi_B)\right]_{f_b} + \sum_{\alpha_r \in \{\alpha_r | f_b\}} \int \left[d\Phi_r R(\Phi)\right]_{\alpha_r}$$

The  $R_{\alpha_r}$  appearing here have singularities regulated by + prescriptions in the FKS framework.

we have

- $\{\alpha_r | f_b\}$  is the set of all singular regions having the underlying Born configuration with flavour structure  $f_b$ .
- $[\ldots]_{\alpha_r}$  means that everything inside is relative to the  $\alpha_r$  singular term: thus R is  $R_{\alpha_r}$ , the parametrization  $(\Phi_B, \Phi_r)$  is the one appropriate to the  $\alpha_r$  singular region

Sudakov FF also carries an  $f_b$  index:

or

$$\Delta^{f_b}(\Phi_n, p_T) = \exp\left\{-\sum_{\alpha_r \in \{\alpha_r | f_b\}} \int \frac{\left[d\Phi_r R(\Phi_n, \Phi_r)\theta(k_T - p_T)\right]_{\alpha_r}}{B^{f_b}(\Phi_n)}\right\}$$

$$\Delta^{f_b}(\Phi_n, p_T) = \prod_{\alpha_r \in \{\alpha_r | f_b\}} \exp\left\{-\sum \int \frac{\left[d\Phi_r R(\Phi_n, \Phi_r)\theta(k_T - p_T)\right]_{\alpha_r}}{B^{f_b}(\Phi_n)}\right\}$$

The Sudakov form factor is a product of elementary Sudakov form factors associated with each radiation region. Technically, one generates radiation by generating a  $k_T$  with each elementary form factor, and choosing the one with the largest  $k_T$  at the end.

#### Single Top

Both initial state and final state radiation is present;



Simplest process with ISR and FSR (simplest because finite without cuts)

We have applied the general formalism given in Frixione, Oleari, P.N. 2007 to single top production (Alioli, Oleari, Re, P.N. 2009).















### Towards automation: the POWHEG BOX

The MIB (Milano-Bicocca) group (Alioli, Oleari, Re, P.N.) is working on an automatic implementation of POWHEG for generic NLO processes.

This framework is being tested in the process  $hh \rightarrow Z + 1$  jet.

### The POWHEG BOX

Build a computer code framework, such that, given the Born cross section, the finite part of the virtual corrections, and the real graph cross section, one builds immediately a POWHEG generator. More precisely, the user must supply:

- The Born phase space
- The lists of Born and Real processes (i.e.  $u \bar{s} \rightarrow W^+ c \bar{c}$ , etc.)
- The Born squared amplitudes  $\mathcal{B} = |\mathcal{M}|^2$ ,  $\mathcal{B}_{ij}$ ,  $\mathcal{B}_{j,\mu_j,\mu'_j}$ , for all relevant partonic processes;  $\mathcal{B}_{ij}$  is the colour ordered Born amplitude squared,  $\mathcal{B}_{j,\mu\nu}$  is the spin correlated amplitude, where j runs over all external gluons in the amplitude. All these amplitudes are common ingredient of an NLO calculation.
- The Real squared amplitude, for all relevant partonic processes.
- The finite part of the virtual amplitude contribution, for all relevant partonic processes.

# Strategy

Use the FKS framework according to the general formulation of POWHEG given in (Frixione, Oleari, P.N. 2007), hiding all FKS implementation details. In other words, we use FKS, but the user needs not to understand it. (Attempts to use the Catani-Seymour method did not work ...) It includes:

- The phase space for ISR and FSR, according to FNO2006.
- The combinatorics, the calculation of all  $R_{\alpha}$ , the soft and coll. limits
- The calculation of  $\tilde{B}$ (spinoff: NLO implementation using the FKS method)
- The calculation of the upper bounds for the generation of radiation
- The generation of radiation
- Writing the event to the Les Houches interface

It works! Lots of more testing needed now ...

#### Case study: Z + jet production

Got virtual matrix elements from MCFM;

Compare NLO predictions obtained with MCFM and the POWHEG BOX

Virtual corrections are the same, but subtraction terms, soft and collinear remnants are all different; non trivial test;











Everything seems to work ...

#### Now compare POWHEG+HERWIG with NLO (red)









Distributions sensitive to more than two jet show noticeably different. All others in agreement with NLO



# Conclusions

- NLO accuracy with Shower MC has become a reality in recent years.
- The POWHEG method is progressing, with new processes being included
- Progress in understanding agreement and differences between MC@NLO and POWHEG
- A path to full automation of POWHEG implementations of arbitrary NLO calculation is open
- Many interesting problems remain to be addressed, and the NLO+Shower community is steadily growing.