Handling Narrow resonances in NLO calculations and NLO+PS generators

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Outline

- Brief reminder on NLO calculation and NLO+PS generators
- Problems with narrow resonances
- "Zero" width approach
- A general approach for finite width
  - Resonance histories: Born and Real case
  - Soft collinear term
- Implementation in the `POWHEG BOX`
- Test case: t-channel single top production
- NLO checks
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Brief reminder of NLO calculations

Besides UV divergences, NLO calculations in QCD display infrared divergences due to the splitting of collinear massless partons and the emission of soft gluons. These are handled in the framework of the subtraction method (Ellis, Ross and Terrano, 1980). Schematically, we write an NLO cross section as

$$\mathrm{d}\sigma = \mathrm{d}\Phi_B (B(\Phi_B) + V(\Phi_B)) + \mathrm{d}\Phi_R\, R(\Phi_R)$$

Introduce a real phase space parametrization: $\Phi_R = \Phi_R(\Phi_B, \Phi_{\mathrm{rad}})$ with a smooth behaviour in the collinear and soft limit, i.e.:

- If two partons become collinear in Φ_R, Φ_B is the phase space for the merged collinear partons.
- If a parton becomes soft, Φ_B is the phase space without that parton.

This assuming that only two partons can become collinear, and only one of the two can become soft. In general cases, R must be separated into a sum of contributions with this properties (i.e. only 1 singular region).

- The phase space is: $\mathrm{d}\Phi_R = \mathrm{d}\Phi_B \, \mathrm{d}\Phi_{\mathrm{rad}}$.
- We call Φ_B the underlying Born of $\Phi_R(\Phi_B, \Phi_{\mathrm{rad}})$

We compute an observable $\mathcal{O}$ (think of a product of theta functions describing a histogram bin) as

$$\begin{aligned}
\langle \mathcal{O} \rangle &= \int \mathrm{d}\Phi_B [B(\Phi_B) + V(\Phi_B)] \mathcal{O}(\Phi_B) + \int \mathrm{d}\Phi_R R(\Phi_R) \, \mathcal{O}(\Phi_R) \\
&= \int \mathrm{d}\Phi_B \left[B(\Phi_B) + V(\Phi_B) + \int \mathrm{d}\Phi_{\mathrm{rad}} R_s(\Phi_B, \Phi_{\mathrm{rad}}) \right] \mathcal{O}(\Phi_B) \\
&+ \int \mathrm{d}\Phi_B \mathrm{d}\Phi_{\mathrm{rad}} [R(\Phi_R(\Phi_B, \Phi_{\mathrm{rad}})) \mathcal{O}(\Phi_R(\Phi_B, \Phi_{\mathrm{rad}})) - R_s(\Phi_R(\Phi_B, \Phi_{\mathrm{rad}})) \mathcal{O}(\Phi_B)] \,.
\end{aligned}$$

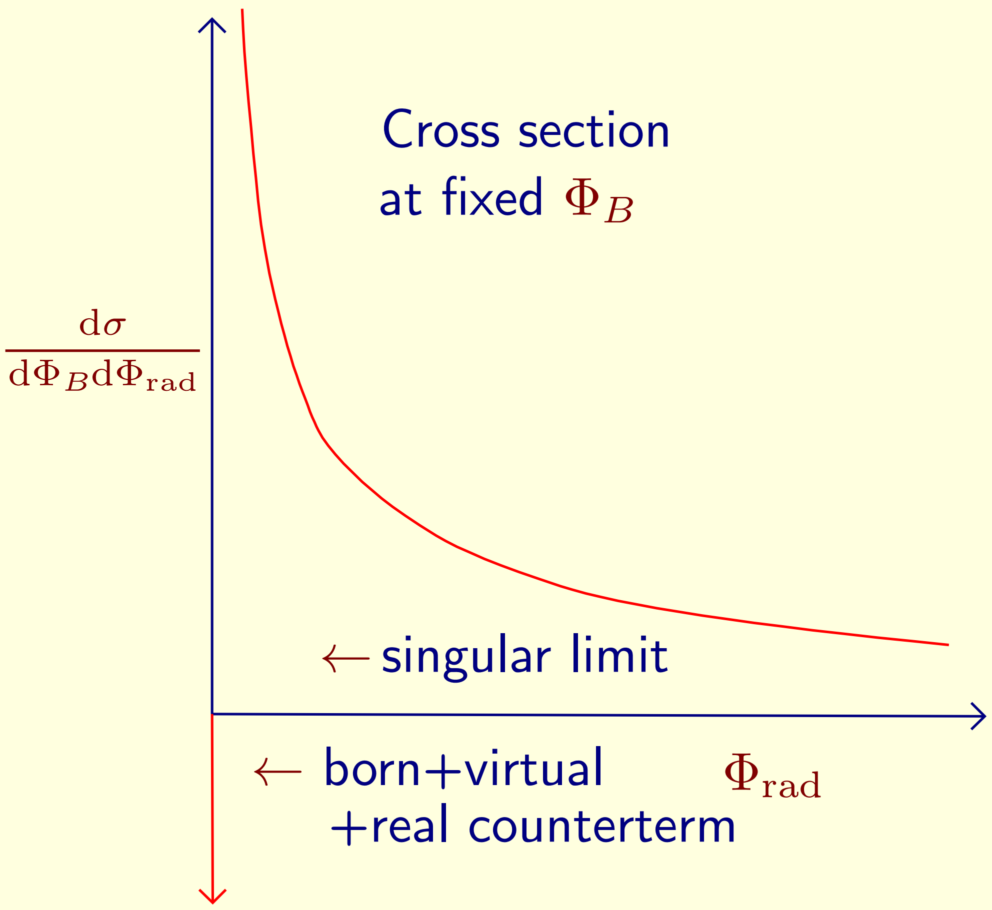
where R_s coincides with R in the soft and collinear limit.

- Only the first term has soft and collinear divergences ($1/\epsilon$, $1/\epsilon^2$ poles) that cancel within the square bracket
- The second term is finite if $\mathcal{O}$ is an IR insensitive observable, i.e. if

$$\mathcal{O}(\Phi_R(\Phi_B, \Phi_{\mathrm{rad}})) \Rightarrow \mathcal{O}(\Phi_B) \quad \text{in the singular limit},$$

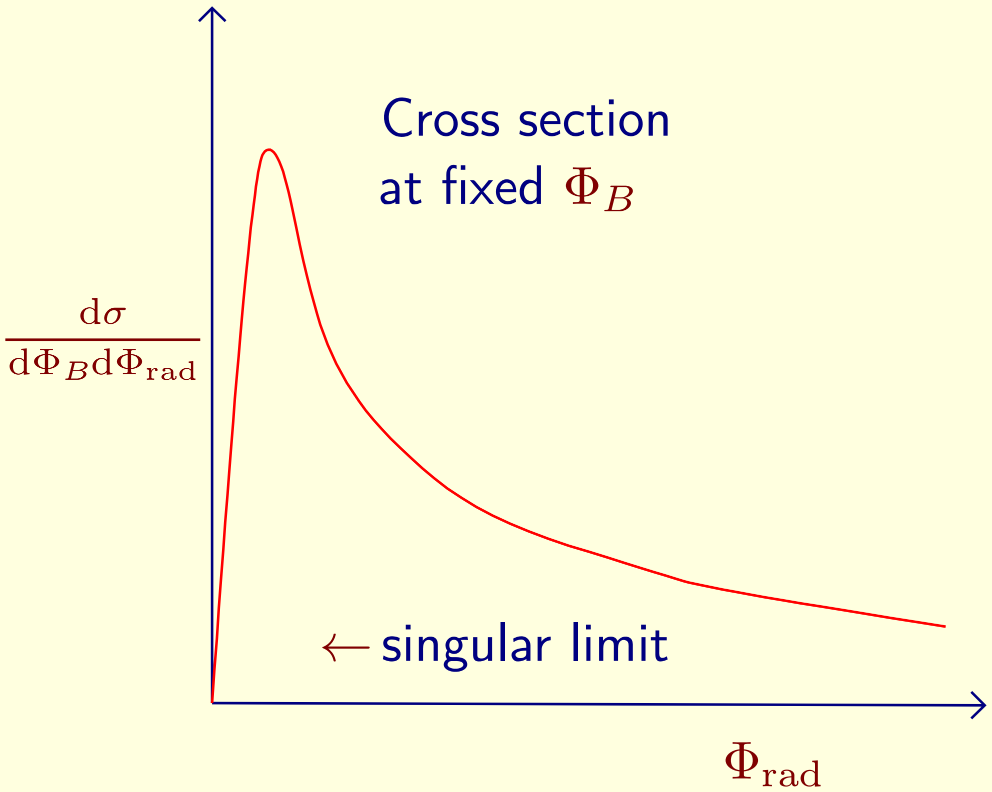
and can be computed safely in 4 dimensions.

NLO calculations: a pictorial representation



At fixed Φ_B, as a function of Φ_R, the cross section is a distribution, i.e. it is divergent in the singular limit, but it has a finite integral over the singular region, i.e. mathematically it is a distribution.

NLO+PS: a pictorial representation



At fixed Φ_B, as a function of Φ_R, the cross section is a smooth function.
Its integral over the singular region is the same as in the NLO cross section.
Differs with respect to the pure NLO due to NNLO and even higher order terms arising from the resummation of leading logarithmic terms.

In the NLO+PS implementations the singularities are tamed by the resummation of Sudakov logarithms. Although the cross section differs from the pure NLO cross section by terms of NNLO and higher, enhanced by Sudakov logarithms near the singular region, the integral in $\Phi_{\rm rad}$ is the same as in NLO.

NLO+PS

$$\begin{aligned} d\sigma &= \tilde{B}(\Phi_B)\exp\left[-\int_{p'_T>p_T}\frac{R(\Phi_B,\Phi'_{\rm rad})}{B(\Phi_B)}d\Phi'_{\rm rad}\right]\frac{R(\Phi_B,\Phi_{\rm rad})}{B(\Phi_B)}d\Phi_B d\Phi_{\rm rad} \\ &+ \left[R(\Phi_B,\Phi_{\rm rad})-R_s(\Phi_B,\Phi_{\rm rad})\right]d\Phi_B d\Phi_{\rm rad} \end{aligned}$$

$$\tilde{B}(\Phi_B)=B(\Phi_B)+V(\Phi_B)+\int R_s(\Phi_B,\Phi_{\rm rad})\,d\Phi_{\rm rad}\,.$$

$$\int \exp\left[-\int_{p'_T>p_T}\frac{R_s(\Phi_B,\Phi'_{\rm rad})}{B(\Phi_B)}d\Phi'_{\rm rad}\right]\frac{R_s(\Phi_B,\Phi_{\rm rad})}{B(\Phi_B)}d\Phi_{\rm rad}=1$$

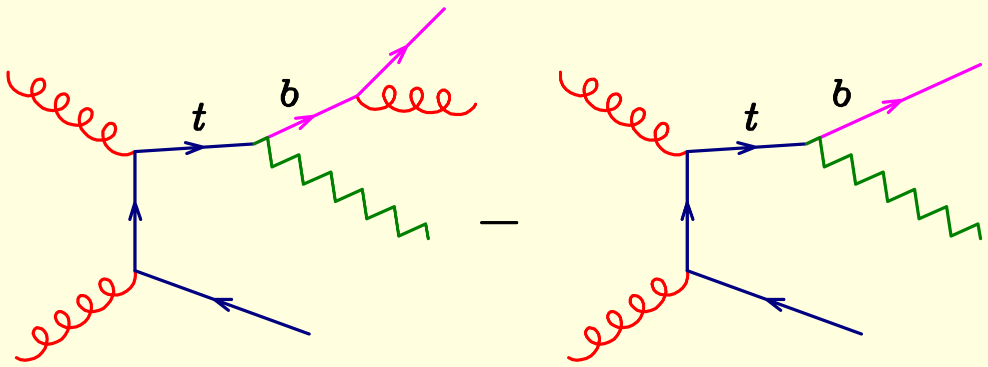
This formula characterizes the hardest emission, both in `MC@NLO` and `POWHEG`. Softer emissions are handled by the shower generator.

As in the NLO, the mapping of the real phase space into an underlying Born is a crucial concept for NLO+PS.

In the `POWHEG BOX`, the NLO subtraction scheme and the NLO+PS implementation are tightly connected.

Problems with resonances: NLO calculations

Standard schemes for NLO calculation fail in the narrow resonance limit.
Example: FKS (Frixione,Kunszt,Signer) in $t\bar{t}$ production



FKS subtraction term kinematics does not preserve the bgW mass.
In the POWHEG BOX scheme: b direction preserved; $W\bar{b}$ recoiling system boosted along b direction and b momentum set to conserve 4-momentum.
Thus: when bgW is on shell, the counterterm is off-shell, spoiling IR cancellation in the narrow width approximation. The same happens with CS (Catani,Seymour) dipoles (W four momentum preserved.)

Message #1:

Current NLO subtraction schemes fail in the narrow width limit

In the top example: the mass of the bg splitting system displaces the top virtuality by an amount m_{bg}^2/E_b (since $\sqrt{E_b^2+m_{bg}^2}\approx E_b+m_{bg}^2/E_b$). Thus, the subtraction works up to

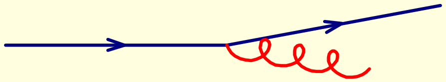
$$\frac{m_{bg}^2}{E_b}\approx\Gamma_t,\quad \text{or} \quad m_{bg}\approx\sqrt{E_b\Gamma_t}\approx 8\,\text{GeV}.$$

This does not look like a severe limitation in practical cases. In fact, NLO calculations of $W^+W^-b\bar{b}$ have been performed by Bevilacqua etal, 2011, and Denner etal, 2012, in the 5-flavour scheme, and Frederix, 2014, massive b.

Yet, a scheme that has a smooth zero width limit is preferrable.

Problems with resonances: PS

Key problem: momentum reshuffling.



Collinear splitting conservers momentum only in the strict collinear limit. Shower Monte Carlo enforce exact momentum conservation by "Momentum reshuffling" (i.e. adjust the momenta by subleading corrections to enforce momentum conservation).

For example (Herwig): If a Final State particle undergoes splitting, and its 3-momentum is kept fixed to balance the 3-momenta of all other FS particles, its energy becomes larger. In order to restore energy conservation, all 3-momenta are rescaled down by a common factor.

If we have a radiating resonance decay, this procedure does not conserve the resonance mass. Hence: in this case, Herwig does momentum reshuffling maintaining the resonance 4-momentum fixed, by rescaling the momenta of the resonance decay products in the resonance rest frame.

Problems with resonances: NLO+PS

POWHEG example:

$$\bar{B}\exp\left[-\int \frac{R}{B}\,\mathrm{d}\Phi_{\mathrm{rad}}\right]\frac{R}{B}\,\mathrm{d}\Phi_{\mathrm{rad}}$$

Here R contains the radiation, and B is the underlying Born kinematics.
The standard POWHEG underlying Born mapping does not preserve resonance virtuality: if R is on shell, B is off shell, R/B LARGE!

More quantitatively: consider for example $t \to bW$; b splits into a bg with mass m^2. The bW mass in the counterterm differs from the original top virtuality by an amount m^2/E_b. So, we expect that

The b jet mass profile is distorted when $m^2_{\mathrm{jet}}/E_b \approx \Gamma_{\mathrm{top}}$.

Message #2:

Current NLO+PS schemes fail in the narrow width limit

Brute force solution: Full $W^+W^-b\bar{b}$ production in POWHEL has been implemented (Kardos,Garzelli,Trocsanyi 2014), using the standard POWHEG BOX mapping. The euristic argument given above would imply unphysical features of jet structure when $m_{\rm jet} \approx \sqrt{\Gamma E} \approx 8\,{\rm GeV}$.

NLO+PS with radiating resonances in `zero width limit`

`POWHEG-BOX-V2` can deal with radiation in resonance decays in the zero-width limit in a fully general way. In order to implement a process one must:

- Specify the resonance and its decay products in the user provided subprocess list. For example:
  ```
  realfl:[ 0, 0,  6, -6, 24,-24,-11, 12, 13,-14,  5, -5, 0]
  realrs:[ 0, 0,  0,  0,  3,  4,  5,  5,  6,  6,  3,  4, 3]
  ```
  represents a real graph for $gg \to (t \to (W \to \bar{e}\nu)\, b\, g)(\bar{t} \to (W^- \to \mu\bar{\nu}))$.
- Virtual corrections should include virtual corrections to resonance decays. In the zero width limit, virtual corrections to production and decay decouple among each other.
- Real correction should yield separately the radiation from the hard interaction (if the radiated parton does not belong to a resonance), and the radiation from each decaying resonance, depending upon `realrs[n]`

Implementation in $t\bar{t}$ production

(Campbell,Ellis,Re,P.N. 2014, **arXiv:1412.1828**, code in the `POWHEG BOX V2`)

Matrix elements from Campbell,Ellis,2012. Narrow resonance decay machinery from `POWHEG BOX V2`. Finite width effects introduced in an approximate way.

Works as follows:

- If radiation comes from a resonance, the underlying Born is constructed in the resonance frame, preserving the resonance 4-momentum and all momenta of particles not arising from the resonance decay.
- Soft radiation does not arise (in the zero width limit) from interference between radiation from different resonances, or from production and a resonance. Thus, soft collinear terms are computed for production and for each radiating resonance decay independently (and in different frames!).

Handling finite width:
the new method

We assume that we have the full cross section for the production of the given final state particles, irrespective of whether they are produced by resonance decays or by other mechanism, and that we have at our disposal the full Born, virtual and real amplitude.

- We consider all possible resonance decay histories that can lead to the given final state.
- We separate the Born and Virtual amplitude into sum of contributions, each one dominant in a single resonance history.
- We separate the Real contribution into a sum of terms, each one of them dominating in a single resonance history, and with no more than one singular region.
- In the real terms, we require that the singular region is compatible with the resonance history. In other words, collinear partons must belong to the same resonance in the resonance history of the given contribution.

In formulae:

$$B_{F_b} = \sum_{f_b \in T(F_b)} B_{f_b}, \qquad B_{f_b} = \Pi_{f_b} B_{F_b}\,,$$

- F_b represent a given final state, irrespective of the resonance history. we call it the bare flavour structure
- f_b represent a given final state and resonance assignment. We call it the full flavour structure.
- $T(F_b)$ represent all possible resonance assignments for the given final state.
- The factors Π_{f_b} satisfy the condition: $\sum_{f_b \in T(F_b)} \Pi_{f_b} = 1$:

$$\Pi_{f_b} = \frac{P^{f_b}}{\sum_{f'_b \in T(F_b(f_b))} P^{f'_b}}\,, \qquad P_{f_b} = \prod_{i \in \mathrm{res}(f_b)} \frac{M_i^4}{(s_i - M_i^2)^2 + \Gamma_i^2 M_i^2}$$

where $\mathrm{res}(f_b)$ represent all resonances in the full flavour structure f_b.

For the real, things are more complex:

$$R_{\alpha_r} = \frac{P^{f_r(\alpha_r)} d^{-1}(\alpha_r)}{\sum_{f'_r \in T(F_r(\alpha_r))} P^{f'_r} \sum_{\alpha'_r \in \mathrm{Sr}(f'_r)} d^{-1}(\alpha'_r)} R_{F_r(\alpha_r)}.$$

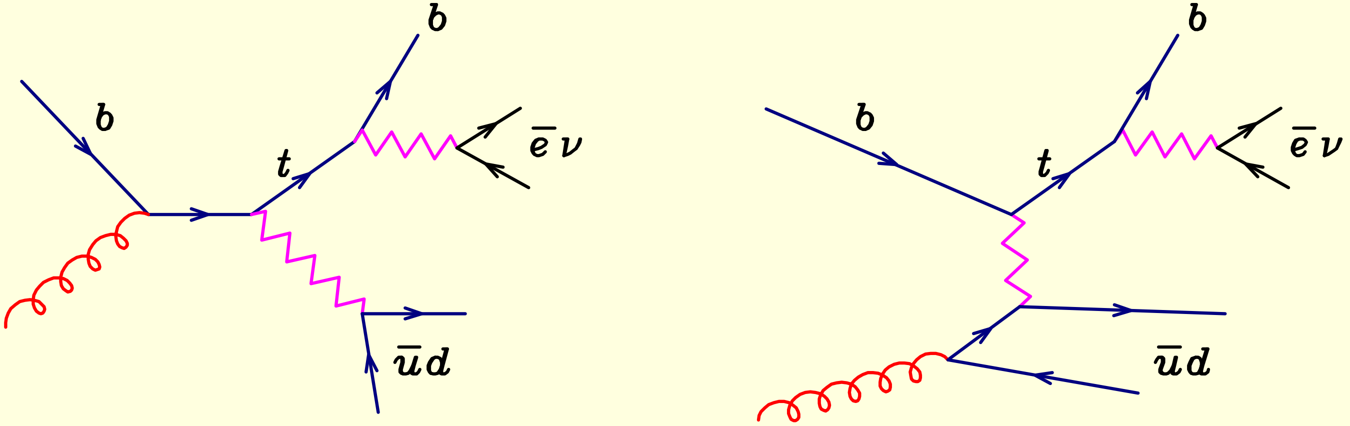
Now:

- α_r labels a contribution to the real that is dominated by a single resonance history, and that has only one collinear singular region.
- $f_r(\alpha_r) \,|\, F_r(\alpha_r)$ represents the full | bare flavour structure of the contribution α_r.
- $\mathrm{Sr}(f_r)$ represent the sets of all α_r with the same f_r
- $d(\alpha_r)$ is a function of the momenta of the collinear partons that vanishes in the collinear or soft limit. Typically:

$$d_{ij} = \left[\frac{E_i^2 E_j^2}{(E_i + E_j)^2} (1 - \cos\theta_{ij}) \right]^b.$$

It is generally frame dependent, but it is Lorentz invariant in the collinear limit.

Example:



The example of two different resonance histories for the same real process in single top production.

In words:

- Each resonance enhancement factor is accompanied by a singular region enhancement factor.
- Singular regions are compatible with the resonance assignment.
- It is easy to show that, with this definition, the sum of all R_{α_r} that have the same bare flavour structure F_b yields the full real contribution for that bare flavour structure.

So, in the separation of the contributions, the following happens: a term R_{α_r} will dominate if the collinear partons of region α_r are the closest in angle, and the corresponding resonance history is the closest to its mass shell.

Having performed this separation into regions, the underlying Born kinematics for a given R_{α_r} is defined in the rest frame of the resonance of the collinear partons, so that the momentum rescaling and boost of the recoil system preserves the resonance 4-momentum.

This feature is already present in the `POWHEG-BOX-V2`.

Notice also that the underlying Born of R_{α_r} is one of the B_{f_b}, since the resonance projection factors for the real become equal to the projection factors for the underlying Born in the singular limit.

Soft-collinear terms

The separation of the divergent soft and collinear terms usually takes place as follows. One writes the phase space for the region where particles i can be collinear to j and soft, as

$$\mathrm{d}\Phi_R = (2\pi)^d \delta\Big(\sum k\Big)[\Pi_{l\neq i}\mathrm{d}\Phi_l]\,\mathrm{d}\Phi_i,$$

and the single particle, d-dimensional phase space is written as

$$\mathrm{d}\Phi_i = \frac{(k_i^0)^{1-2\epsilon}}{2(2\,\pi)^{3-2\epsilon}}\,\mathrm{d}k_i^0\;\mathrm{d}\,\Omega_i^{3-2\epsilon},$$

Soft terms are separated first by defining $\xi = 2k_i^0/\sqrt{s}$, and writing:

$$(k_i^0)^{1-2\epsilon}\,\mathrm{d}k_i^0 \Rightarrow \xi^2\left(\frac{1}{\xi^{1+2\epsilon}}\right)\mathrm{d}\xi, \qquad \xi^{-1-2\epsilon} = \frac{-1}{2\epsilon}\delta(\xi) + \left(\frac{1}{\xi}\right)_+ - 2\epsilon\left(\frac{\log\xi}{\xi}\right)_+.$$

The $\delta(\xi)$ term singles out the soft term.The soft contribution becomes

$$I_{s,\alpha_r} = -\frac{1}{2\epsilon}\,\mathrm{d}\Phi_B \int \frac{(s)^{1-\epsilon}}{(4\,\pi)^{3-2\epsilon}}\,\mathrm{d}\,\Omega^{3-2\epsilon} \lim_{\xi\to 0}\,[\xi^2 R_{\alpha_r}]$$

At this point one can sum over all the α_r that share the same soft singularity, and recover the soft approximation to the real cross section, given by the soft eikonal formula, and the soft integral can be easily performed.

However:
In order for this to work, k^0 must have the same meaning for all soft contributions, at least in the soft limit. This means that in the soft limit the soft phase space must be the same for all singular regions.

In our case, this is no longer true. We require that subtractions are performed in the frame of the resonance that owns the emitting parton. Thus, several different definitions of k^0 are used, and one can no longer conclude that the sum of all soft contributions yields the full R.

We deal with this problem using the following trick. We rewrite

$$
\begin{aligned}
I_{s,\alpha_r} &= -\frac{1}{2\epsilon}\,\mathrm{d}\Phi_B \int \frac{(k_{\mathrm{res}}^2)^{1-\epsilon}}{(4\,\pi)^{3-2\epsilon}}\,\mathrm{d}\,\Omega^{3-2\epsilon} \lim_{\xi_{\mathrm{res}}\to 0}\,[\xi_{\mathrm{res}}^2 R_{\alpha_r}] \\
&= \mathrm{d}\Phi_B \frac{1}{\Gamma(1-2\epsilon)} \int \mathrm{d}\Phi_i \frac{e^{-\xi_{\mathrm{res}}}}{\xi_{\mathrm{res}}^2} \lim_{\xi\to 0}\,[\xi_{\mathrm{res}}^2 R_{\alpha_r}] \\
&= \mathrm{d}\Phi_B \frac{1}{\Gamma(1-2\epsilon)} \int \mathrm{d}\Phi_i e^{-\xi_{\mathrm{res}}}\,\tilde{R}_{\alpha_r}
\end{aligned}
$$

ξ_{res} being the ξ defined in the radiating resonance frame. We used the identity

$$\int_0^\infty \mathrm{d}\xi \xi^{-1-2\epsilon}\,e^{-\xi} = \Gamma(-2\epsilon) = \frac{\Gamma(1-2\epsilon)}{-2\epsilon},$$

and the Lorentz invariant soft linearization of R_{α_r}:

$$\tilde{R}_{\alpha_r} = \frac{1}{\xi^2} \lim_{\xi\to 0}\,[\xi^2 R_{\alpha_r}].$$

Now the expression for I_{s,α_r} is all Lorentz invariant, except for the factor $e^{-\xi_{\mathrm{res}}}$.

- We replace $e^{-\xi_{\rm res}}$ with $e^{-\xi}$. The formula can then be turned into the standard formula for soft divergences, and can be integrated as usual.
- We add back the difference $e^{-\xi_{\rm res}} - e^{-\xi}$. This difference does not have soft singularities. It still has collinear singularity need to be worked out analytically. Their computation leads to an analytic form for the divergent part, plus an analytic expression for a finite part, plus a finite reminder to be integrated numerically using the soft phase space weighted with the $e^{-\xi_{\rm res}} - e^{-\xi}$ difference, and that does not pose any problem in the narrow width limit.

At the end of this procedure:

- We have a new formula for the soft-collinear terms, that we implement in the `POWHEG BOX`.
- We have an extra finite term, that can be easily obtained by a numerical integration in the soft phase space, of an expression proportional to $e^{-\xi_{\rm res}} - e^{-\xi}$.

POWHEG BOX implementation

All this has been implemented in a fully general way in a new version of the `POWHEG BOX`. Now:

- As an input, the user provides the Born, Virtual and real matrix elements for the bare flavour structures, and the full flavour lists for the Born process and real processes. (We are planning to implement soon the automatic generation of the full flavour structures, given only the bare ones).
- For each Born resonance structure, an independent phase space sampling is set up automatically that probes the resonance peaks.
- The set of α_r is determined by the `BOX`, including the regular contributions.
- P weights are computed and included automatically.
- Radiation is handled using the already present (zero width case) mappings.

Testing

We have tested the system for the process of t-channel single top production, with massless b quark.

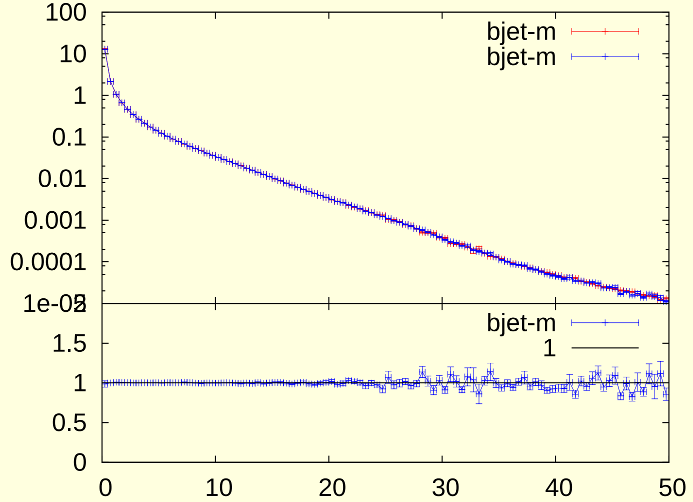
First test:

- Compute the NLO result, at fixed coupling, ignoring resonances at first, and then using the resonance features discussed here.
- We label the two generators as `no-res` and `res` in the following. Insisting enough with statistics, we must get exactly the same result.
- In the single top case, this is more easily done if the "no resonances" implementation uses a resonance aware, importance sampling Born phase space.

- NLO test plots: global suppression factor (mostly to avoid collinear b's)

$$\left(\frac{M_{e\nu}^2}{(M_{e\nu}^2+40^2)}\right)^3 \times \frac{20}{\exp((y_b-y_W)^2)+20}$$

- No virtuals (irrelevant for the check)
- Top defined a $e\nu b_{\rm jet}$
- Jets: anti-k_T, $R=0.5$;
- wct: mass of hadronic fs system excluding b jet within 2 GeV from W mass (enhanced regular W^+ production)
- In the plots:
  - red: `res`
  - blue: `no-res`


bjet-m
bjet-m
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1
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1
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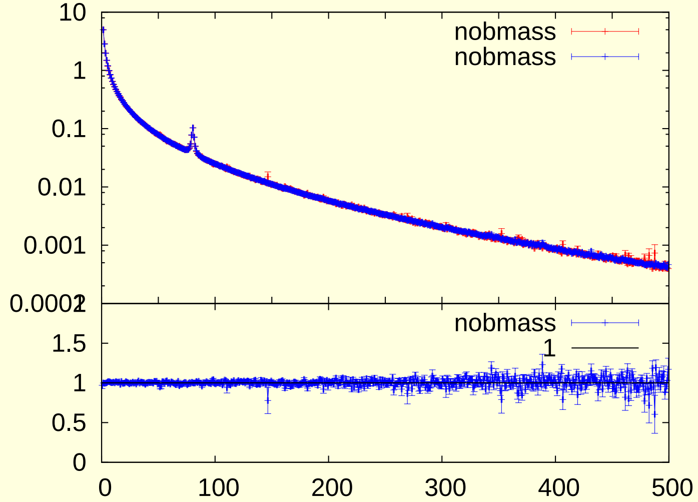
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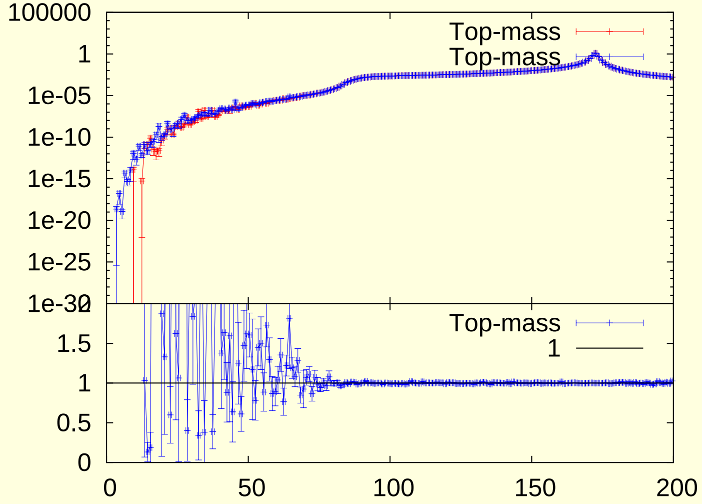
Top-mass
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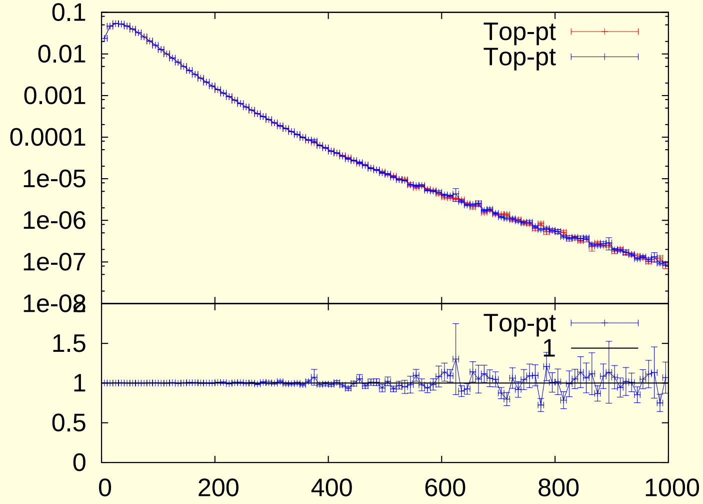
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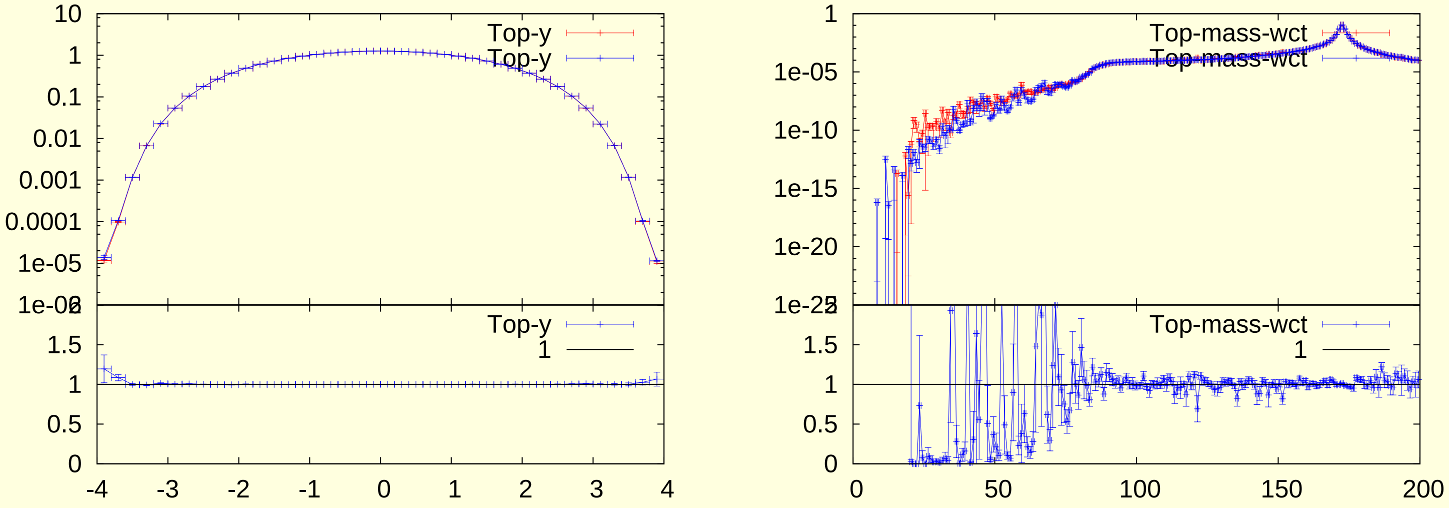
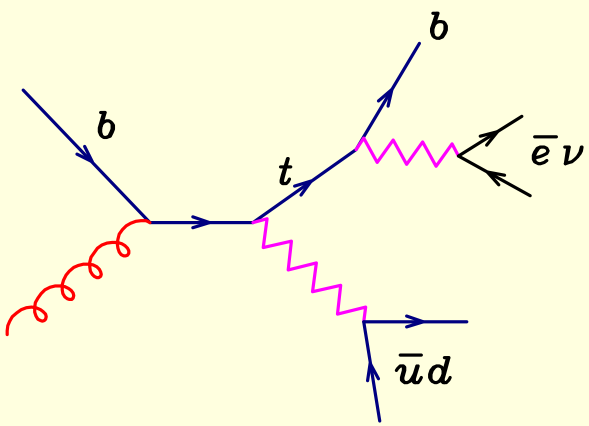


The second plot enhances the graph:



Non-resonant aware calculation undershoots low top mass end. However, the region still drifts towards the red curve when statistics is increased, pointing to a poor importance sampling when statistics is poor.

Non resonant aware calculation: ≈ 3 times slower. However, in this case the Born importance sampling is easy (only 1 resonance history at Born level)

Full Simulation

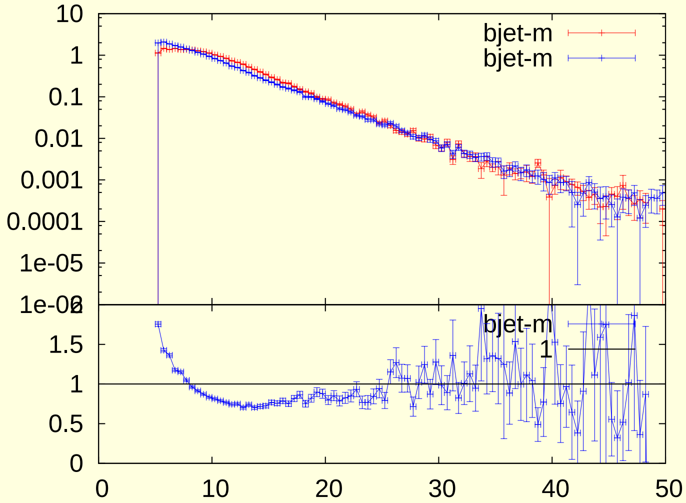
For the generation of events, we have interfaced POWHEG to Pythia 8, using both the traditional code (no resonances recognized) and the new, resonance aware code.

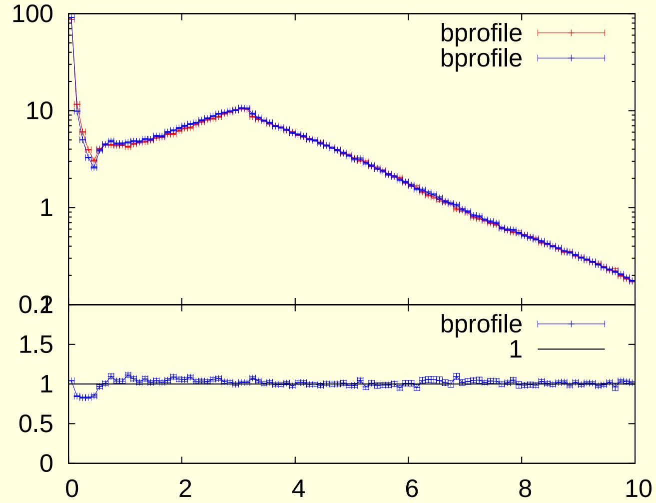
No resonances:

- No resonance information was included in the Les Houches file.
- Pythia radiation was vetoed using the standard Les Houches mechanism

With resonances:

- The hardest radiation from production and from the resonance decay are both kept (normally POWHEG keeps the hardest of the two).
- Radiation in production is normally vetoed by PYTHIA not to be harder than that of POWHEG.
- Radiation in resonance decay by PYTHIA is vetoed by hand, if harder than POWHEG radiation in decay, the shower is repeated on the same event.

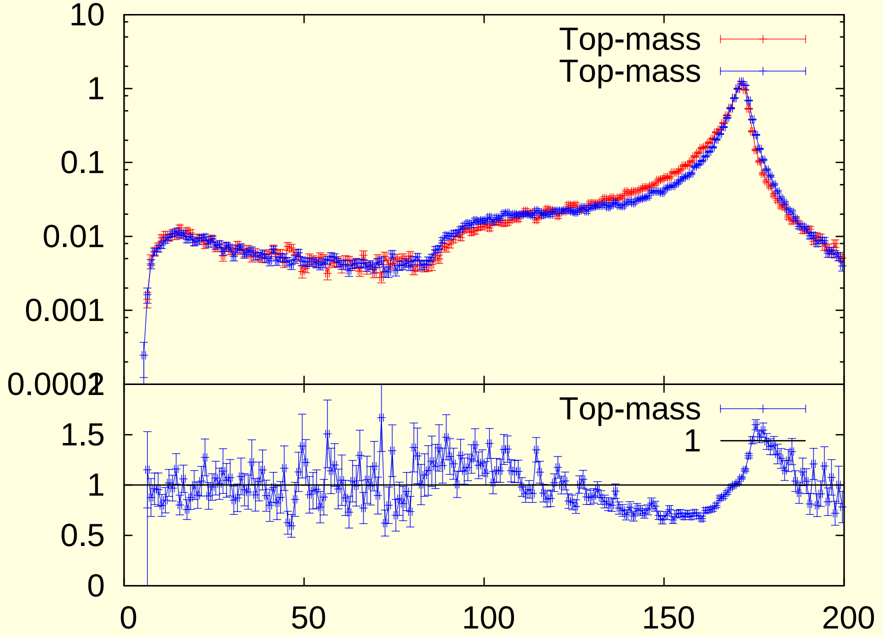




The b jet is the jet containing the hardest b hadron.

There are visible effects in the $b - \mathrm{jet}$ mass distribution.

The `bprofile` distribution is a histogram of the hadronic transverse energy flow versus the ΔR distance from the b jet.



Some distortion in the top mass profile is also seen.

Conclusion

- A new method for the NLO calculation, and for NLO+PS generation, that deals with resonances and remains consistent in the small-width limit has been conceived and implemented in the `POWHEG BOX`.
- Preliminary studies on single top production show noticeable differences when this method is used with respect to the `no-res` (i.e. no resonance aware) method.
- The new method has a considerable advantage, in terms of speed, with respect to the non-resonance aware method (order of a factor of 10 in the generation of events).
- Still to be checked: whether a fudged resonance assignment in the `no-res` generator improves the agreement with `res` results.