Heavy quark radiation in NLO+PS POWHEG generators

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Outline

- Radiation from a heavy quark
- Implementation of a new algorithm
- Preliminary results
- Conclusions

Radiation from a heavy quark - Motivations

Bottom quark physics at LHC:

- Aside the very abundant direct production, that is exploited for flavour physics studies, bottom is used to identify top particles and to study their properties. **Bottom fragmentation function** may have a relevant phenomenological impact on the physics of the top.
- Detection of the Higgs boson in its bb~ decay mode
- In searches for new physics, bottom also appears often produced in association with new-physics objects.

Electroweak shower from massive charged particle

- The same formalism can be employed also for describing photons radiation from massive charged fermions. Application for electroweak precision studies (such as H -> τ+τ-, ...)

Radiation from a heavy quark - Introduction

Fixed Next-to-Leading order calculations

Full mass effects are taken into account. The mass of the heavy quark acts as a regulator of the collinear singularities and fixes the scale of the process (single scale).

Hadroproduction: *Nason, Dawson, Ellis, NP B*327 (1989) 49, *NP B*303 (1988) 607

*Beenakker, van Neerven, Meng, Schuler, Smith, NP B*351 (1991) 507

Photoproduction: *Nason,Ellis, NP B*312 (1989) 551

*Smith, van Neerven, NP B*374 (1992) 36

High-p_T regimes

In cases when the transverse momenta involved in the production of a heavy quark is large compared to its mass, as, for example, in **high-energy e+e− annihilation**, or in **production at large transverse momentum in hadronic collisions**, heavy quark (bottom) **can in part behave as a light parton and give rise to a hadronic jet**.

Large logarithms of the heavy quark transverse momentum divided by its mass arise

→ Need for a massless resummed approach!

Radiation from a heavy quark - Introduction

FONLL: [*Cacciari, Greco, Nason, JHEP* 9805 (1998) 007]

Matches fixed order calculation with resummation of the large logarithms at Next-to-Leading Logarithmic level.

- **Pros**: combine full mass dependence with multiscale resummed approach; scale uncertaintes are reduced at high-p_T. Successfully employed for LHC physics [*Cacciari, Frixione, Houdeau, Mangano, Nason, and Ridolfi, JHEP* 10(2012) 137].
- **Cons**: it provides "only" the double-differential (p_T and rapidity), **single inclusive** distibution. It is not an exclusive event generator.

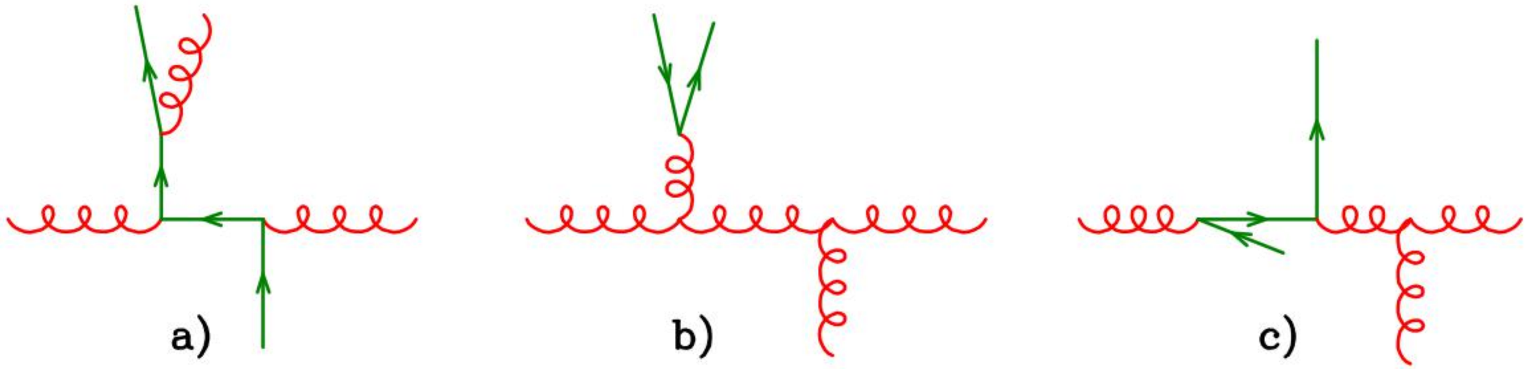
Parton Showers Approach

Heavy flavours are **treated as light flavours** with a **cut-off scale** of the order of the heavy quark mass. Some mass effects included with ad-hoc variations of the splitting kernels.

- This approach is consistent at Leading Logarithmic level and fully exclusive.
- It is difficult to deal correctly with mass effects and account at the same time for the resummation of collinear logarithms.

Radiation from a heavy quark - Large Logs

Contributions potentially affected by large logarithmic enhancements of the heavy quark transverse momentum divided by its mass:



a) Radiation from heavy quark: real gluon emission from external heavy quark leg. The collinear singularity of the massless case is replaced by a logarithm of p_T/m (*dead cone* effect)

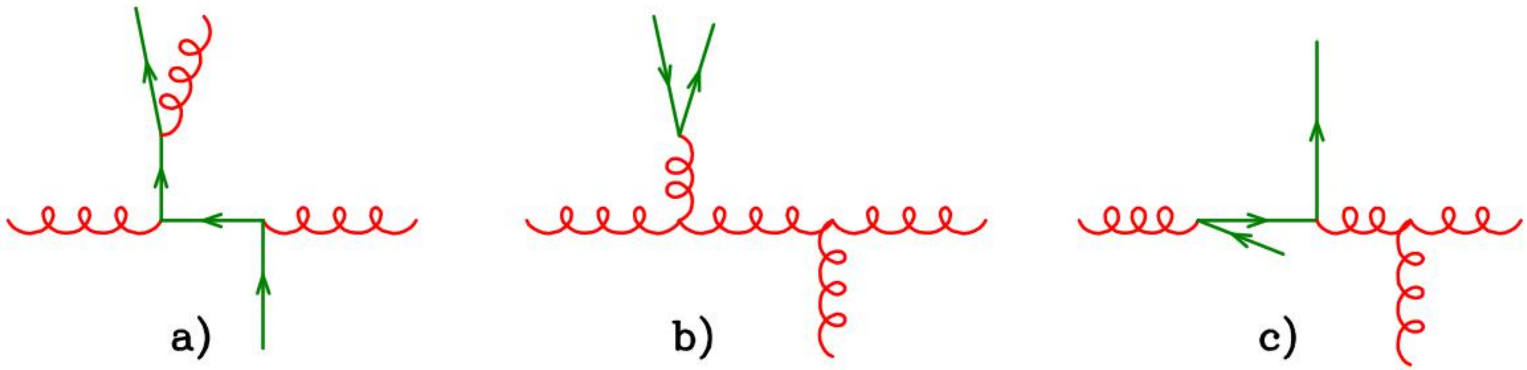
b) Gluon splitting: production of heavy quark-antiquark pair via final state gluon splitting

gg -> gg follows by g -> QQ_{bar}

c) Flavour excitation: splitting of an initial state gluon into a heavy quark-antiquark pair, where one of the two quarks is scattered at large transverse momentum via gluon.

Radiation from a heavy quark - Large Logs

Contributions potentially affected by large logarithmic enhancements of the heavy quark transverse momentum divided by its mass:



Gluon splitting and flavour excitation belong to a different class of production mechanisms:

- the underlying Born does not belong to the production of a heavy quark pair;
- difficult to handle in a rigorous manner in NLO+PS generators;
- specific of heavy quark pair production process.

Here we focus on **radiation from heavy quark at NLO+PS level**

- treated consistently as a new "quasi" collinear singular region in POWHEG
- improved description of the radiative content of the heavy quark fragmentation function
- it shares the same structure as photon radiation from a charged massive particle.

POWHEG developments

- Early POWHEG generator: **hvq** [*Frixione, Nason, Ridolfi* 2007] for c, b and t. **Heavy quarks treated as heavy:** no collinear singularities from heavy quark emissions were considered. **Only one singular region: R_{ISR}.**

- In 2012: alternative treatment of radiation from heavy fermions (hvqaslight option), introduced in the framework of W production with electroweak corrections [*Barzè, Montagna, Nason, Nicrosini, Piccinini JHEP* 1204 (2012) 037]. A **phase space mapping appropriate to massive fermions was introduced**, in order to separate out also a region $R_{FSR,q}$ for each massive quark q that can radiate gluons.

- In 2015: first resonance aware generator RES [*Ježo, Nason*, JHEP 1512 (2015) 065]. Applications: single top and successively top pair production and decay (with massive b's) [*Ježo, Lindert, Oleari, Pozzorini, Nason EPJ C76* (2016) 12, 691]

- Here we present a new mapping for massive fermions and its full implementation in POWHEG-BOX-RES.

WARMUP: FKS mapping in POWHEG

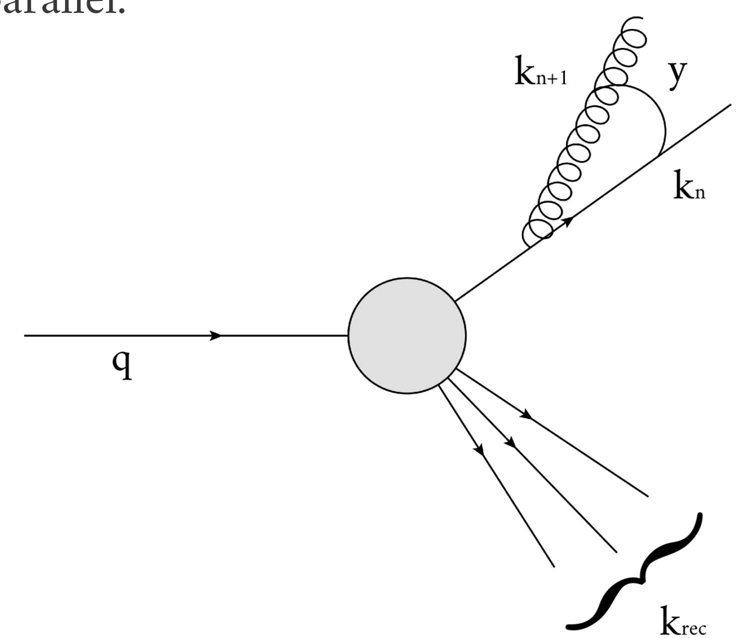
In the subtraction method, one introduces a parametrisation of the real phase space of the form

$$\Phi_{R}=\Phi_{R}(\Phi_{B},\Phi_{\text{rad}}) \longrightarrow d\Phi_{R}=d\Phi_{B}d\Phi_{\text{rad}}$$

(factorization)
Born X extra parton

In the FKS formalism, one separates **different singular regions** which factorise in the collinear limit.

The idea is to associate the extra parton to an emitter (massless) parton in the Born kinematics. The collinear limit corresponds to the emitter and the radiated parton becoming parallel.



FKS parametrisation
(in the partonic CM-frame)

$$\xi=\frac{2k_{n+1}^{0}}{q} \qquad y=\frac{\vec{k}_{n}\cdot\vec{k}_{n+1}}{\left|\vec{k}_{n}\right|\left|\vec{k}_{n+1}\right|}$$

soft limit

collinear limit

WARMUP: Real to Born map

The map **must preserve**:

- the CM energy-momentum

$$q = \sum_{i=1}^{n+1} k_i = \sum_{j=1}^{n} \bar{k}_j$$

- all mass shell relations

$$k_i^2 = \bar{k}_i^2 = m_i^2, \quad i = 1, \ldots, n$$

$$\boxed{k_n^2 = \bar{k}_n^2 = 0}$$

Barred notation: $\Phi_R = \{k_i\}_{i=1}^{n+1}, \quad \Phi_B = \{\bar{k}_i\}_{i=1}$

Step-by-step construnction

1. The emitter and the emitted partons are merged together into a single parton (same flavour of the emitter) with momentum k parallel to the sum of the two.
2. To restore mass shell relation, a **boost Λ** along the direction of the 3-momentum $\mathbf{k}$ is employed.
3. The Born emitter momentum is constructed as

$$\bar{k}_n = \Lambda k + (1 - \Lambda) q = q - \Lambda k_{\mathrm{rec}} \Longrightarrow \boxed{(q - \Lambda k_{\mathrm{rec}})^2 = 0}$$

this fixes the β parameter of the boost

4. The recoil system is boosted to restore CM energy-momentum conservation.

Massive Emitter: the "inversion problem"

In practice, what it is really needed is the inverse map

$$\Phi_B = \{\bar{k}_i\}_{i=1}^{n}, \Phi_{\rm rad} = \{\xi, y, \varphi\} \qquad \longrightarrow \qquad \Phi_R = \{k_i\}_{i=1}^{n+1}$$

This kinematical problem admits the following resolutive strategy:

1. the modulus of $\mathbf{k_{n+1}}$ is given by $\left|\vec{k}_{n+1}\right| = \frac{q}{2}\xi$
2. the modulus of $\mathbf{k_n}$ must satisfy the energy conservation constraint
$$\boxed{q = k_{n+1}^0 + \sqrt{\vec{k}_n^{\,2} + m^2} + \sqrt{\vec{k}_{\rm rec}^{\,2} + M_{\rm rec}^2}}$$
3. the directions of the 3-momenta $\mathbf{k_n}$ and $\mathbf{k_{n+1}}$ are determined by the condition
$$\vec{k}_n + \vec{k}_{n+1} \parallel \vec{\bar{k}}_n$$
4. the inverse boost Λ^{-1} is applied to build the remaining momenta

Critical point: the inversion for $\mathbf{k_n}$ admits two solutions!

$$k_n^{(\pm)} = \frac{-(2\bar{k}_n^{\,0} - q\xi)\xi y \pm (2-\xi)\sqrt{(2\bar{k}_n^{\,0} - q\xi)^2 - m^2\xi^2(1-y^2) - 4m^2(1-\xi)}}{(2-\xi)^2 - \xi^2 y^2}$$

The double-covered structure in the ξy-plane

We analyzed the structure of the physical solutions in the ξy-plane

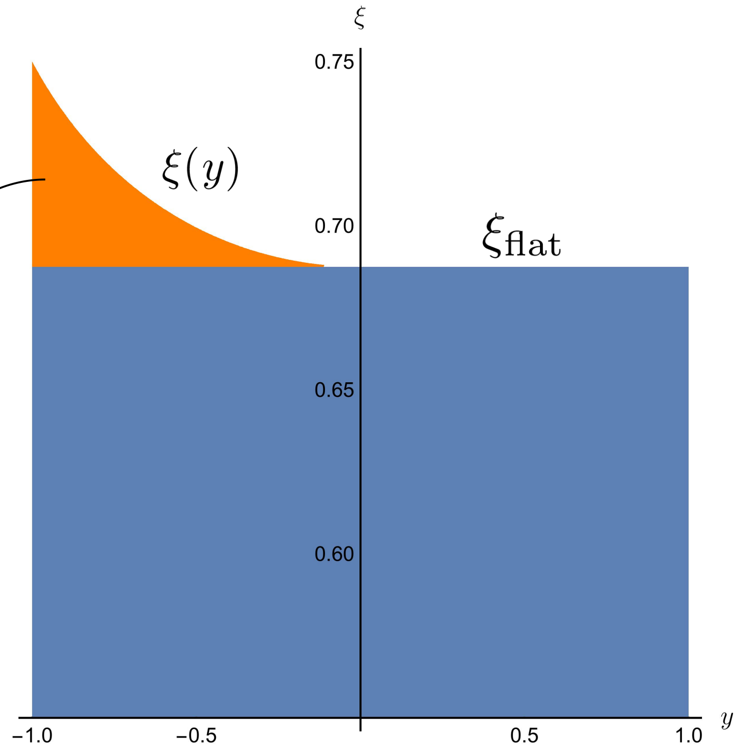
$$k_n^{(+)}: \quad y > 0, \quad \xi < \xi_{\text{flat}} = 2\frac{\bar{k}_n^0 - m}{q - m}$$

$$y < 0, \quad \xi < \xi(y) = 2\frac{\bar{k}_n^0 q - m^2 - \sqrt{(q - \bar{k}_n^0)^2 - \vec{k}_n^{\,2} y^2}}{q^2 - m^2 + m^2 y}$$

$$k_n^{(-)}: \quad y < 0, \quad \xi_{\text{flat}} < \xi < \xi(y)$$

In this region, two physical configurations correspond to the same (y,ξ) point

The one-to-one correspondence is lost!

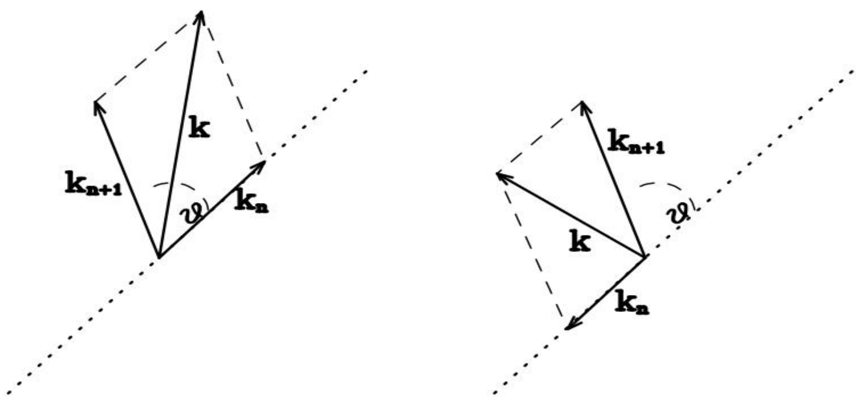


Our solution: a mirror game

We observe that the two solutions are related

$$k_n^{(+)}(y,\xi) = -k_n^{(-)}(-y,\xi)$$

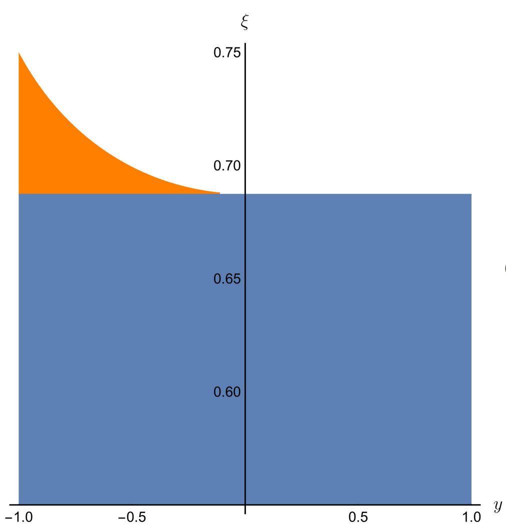
This allows a physical interpretation of the negative values of $k_n^{(+)}$ solution



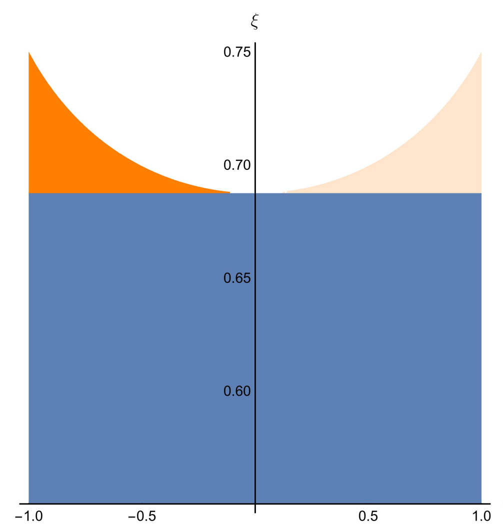
$$y > 0, \quad \xi_{\rm flat} < \xi < \xi(y)$$

Solution: pick only the $k_n^{(+)}$ solution and allow for negative values

one-to-one correspondence restored!



extended region



Beware: here y does not retain its physical meaning

$$y_{\rm phy} = -y$$

Jacobian singularity and Dalitz plot

Associated to the mapping of the radiation phase space, the jacobian

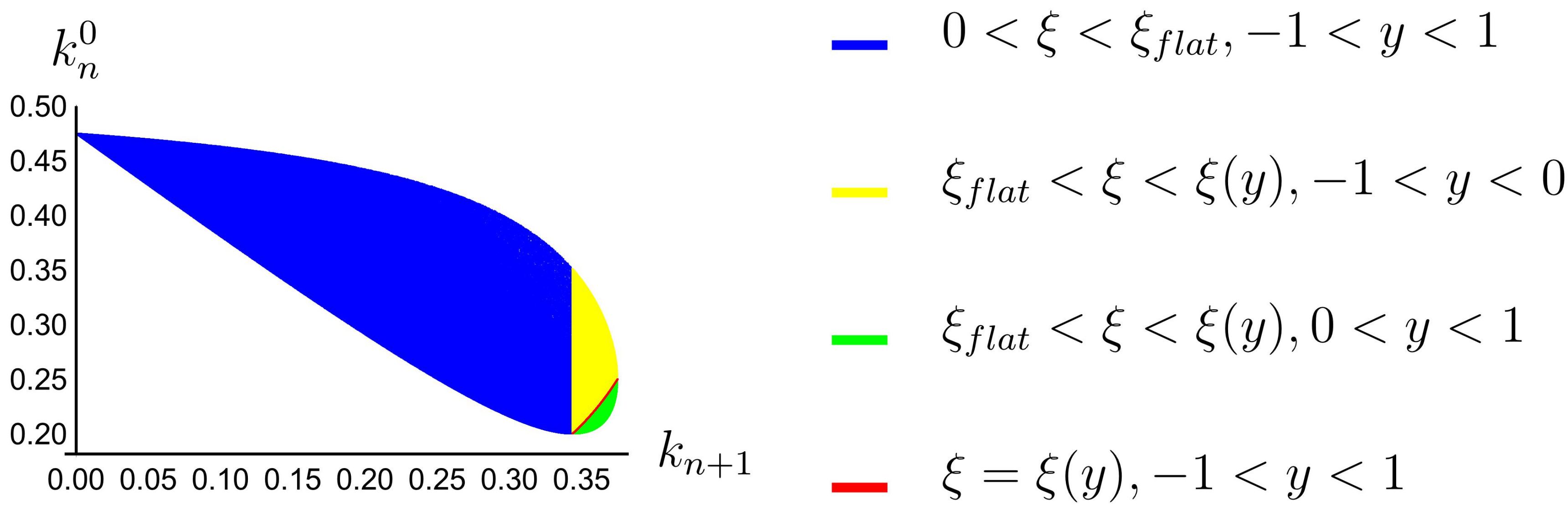
$$d\Phi_R = d\Phi_B J(\xi, y, \varphi) d\xi \mathrm{d}y\mathrm{d}\varphi$$

$$\boxed{J(\xi, y, \varphi) = \frac{q^2}{(4\pi)^3}\xi \left|\frac{\vec{k}_n^{\,3}}{\vec{\bar{k}}_n}\right| \frac{1}{k_n^0(\bar{k}_n^0 - k_{n+1}^0) - m^2(1 - k_{n+1}/q)}}$$

The denominator vanishes on the upper curve ξ=ξ(y)

The associated **singularity** is integrable (it behaves asymtotically as a square-root)

Its integration can be accomodated by the importance sampling technique



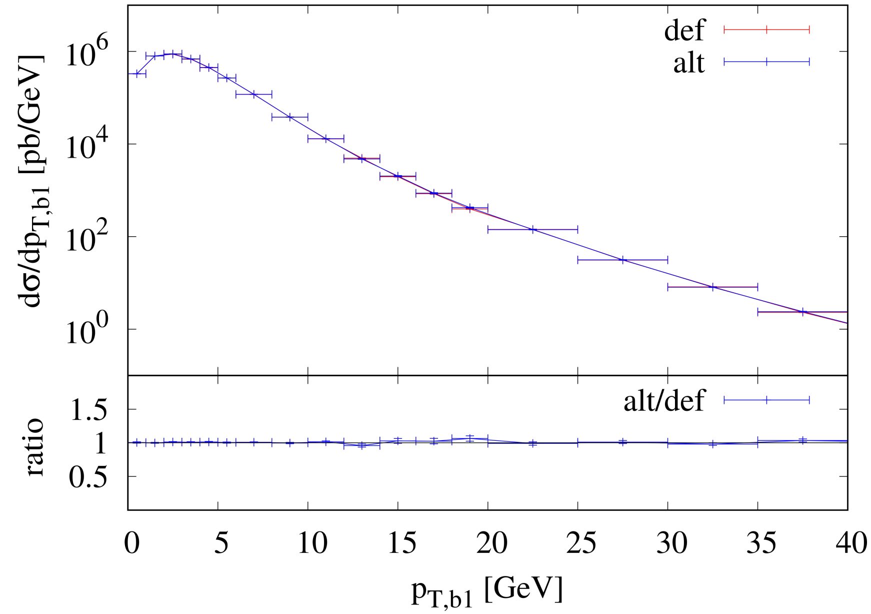
Validation - NLO plots

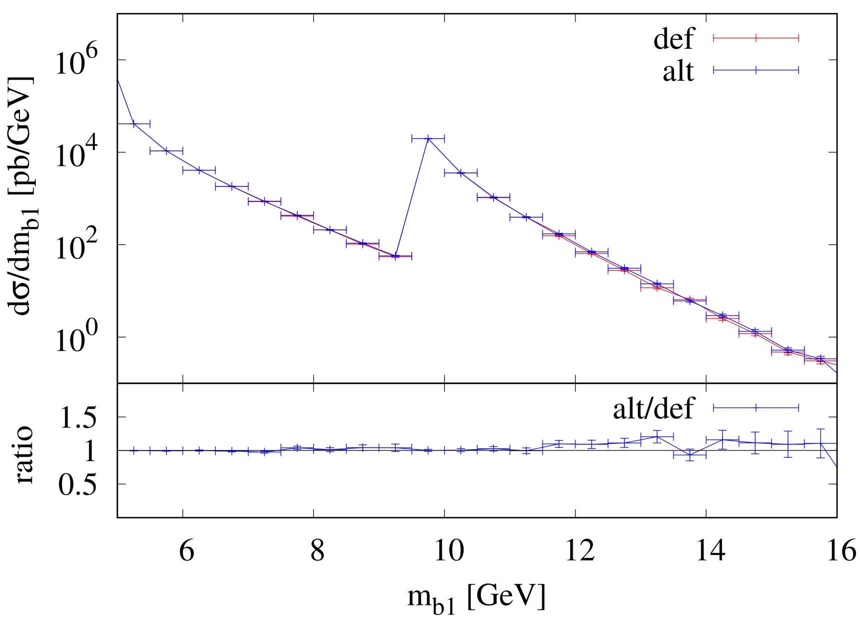
Consistency tests at NLO level:

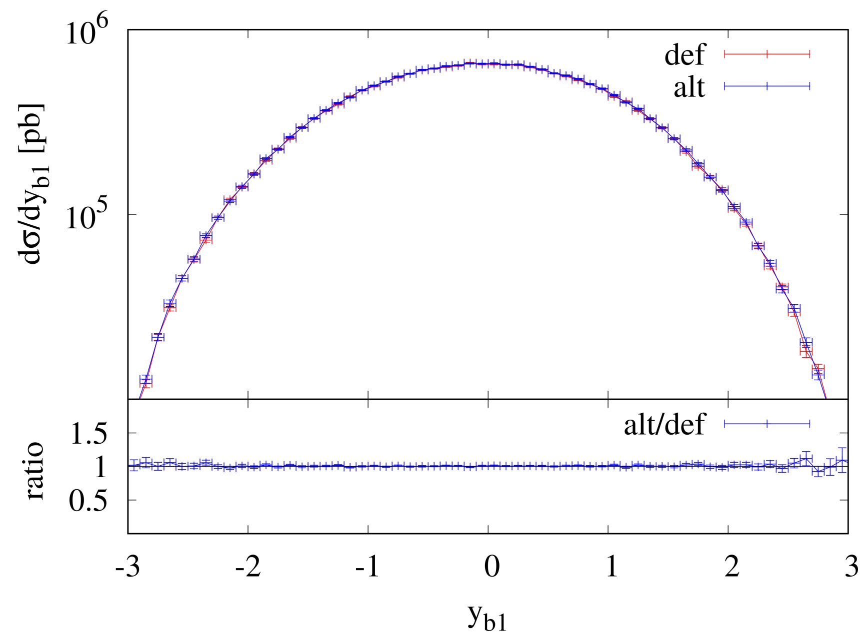
- cancellation of divergences
- total cross section
- NLO distributions

def: old implemenation

alt: new implemention







Generation of radiation - POWHEG

POWHEG **master formula** for generation of radiation

$$d\sigma_{\rm NLO} = \bar{B}(\Phi_B) d\Phi_B \left[\Delta_{\rm NLO}(\Phi_B, 0) + \sum_\alpha \int \frac{\left[d\Phi_{\rm rad} \Delta_{\rm NLO}(\bar{\Phi}_B, K_T(\Phi_R) R(\Phi_R) \right]_\alpha^{\bar{\Phi}_B = \Phi_B}}{B(\Phi_B)} \right]$$

NLO cross-section integrated over radiation variables

sum over singular regions

NLO Sudakov Form factor

$$\Delta_{\rm NLO}(\Phi_B, p_T) = \exp\left[-\sum_\alpha \frac{\left[d\Phi_{\rm rad} R(\Phi_R) \Theta(K_T(\Phi_R) - p_T \right]_\alpha^{\bar{\Phi}_B = \Phi_B}}{B(\Phi_B)} \right]$$

Definition of the hardness scale for massive emitter

In the massless case the "hardness" of the process is associated to the transverse momentum of radiation.

In the massive case, a greater value of the gluon virtuality is allowed.

We rely on the definition $\boxed{K_T^2(\xi, y) = 2\frac{k^0}{p^0} p \cdot k = \frac{q^2}{2} \xi^2 (1 - \beta y_{\rm phy})}$ **(Barzè et al 2012)**

Generation of radiation - Implementation

- In our mapping, the hardness scale K_T^2 is a complicated function of the ξ, y variables. As it stands, following the standard **veto algorithm** approach for the generation of radiation is an extreme difficult task.
  Analitical integration with the K_T^2-theta constraint is really hard!

- It turns out that we are allowed to perform a change of variable from y to K_T^2 at fixed ξ (thanks to monotonic properties of K_T^2).

- We define an upper bound function in the new variable (ξ, K_T^2) which incorporates the jacobian factor of the transformation.

$$U(\xi,t)d\xi\mathrm{dt} \geqslant \underbrace{\frac{R}{B}}_{\frac{1}{K_T^2}} \underbrace{J(\xi,y)}_{\xi} \underbrace{\frac{\partial y}{\partial k_T^2}}_{\frac{1}{\xi^2}} d\xi\mathrm{dt} \quad \Longrightarrow \quad \boxed{U(\xi,K_T^2)=\frac{1}{\xi K_T^2}}$$

soft-collinear behaviour

- We obtain an improvement of the algorithm: both integration and inversion performed analitically! (we skip some tedious details)

Treatment of jacobian singularity

Again in trouble: we forgot the jacobian singularity!

$$J(\xi, y) \sim \frac{1}{\sqrt{\xi(y) - \xi}}$$ near the upper limit curve $\xi(y)$

Source of inefficiency!
It spoils the simplicity of the upper bound function

Observation

The enhancement arises in a region of the radiation phase space far away from soft and collinear singularities: ξ is large and y_{phy} is negative.

POWHEG remnant mechanism

$$R = \underbrace{F}_{\text{damp factor}} R + (1 - F)R = R_s + R_f$$

- "Btilde" events generated according to the NLO Sudakov with R_s
- "Remnant" events generated according to R_f (with hit-or-miss)

Preliminary results - Comparison studies

Comparisons between the new implementation (**alt**) with the old one (**def**)

- **Study cases**: HVQ 200 GeV pp collisions, 1.96 TeV p p~ collisions

  b_bbar_4l in 13TeV pp collisions

- **Parameters** m_b=4.75 GeV, NNPDF3 pdf set

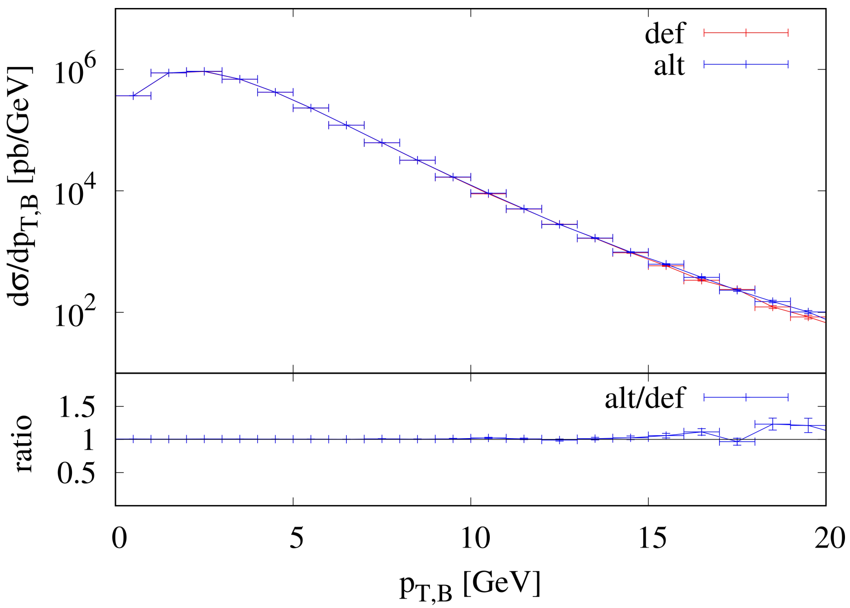
- **Parton Shower:** PYTHIA v. 8.2.23

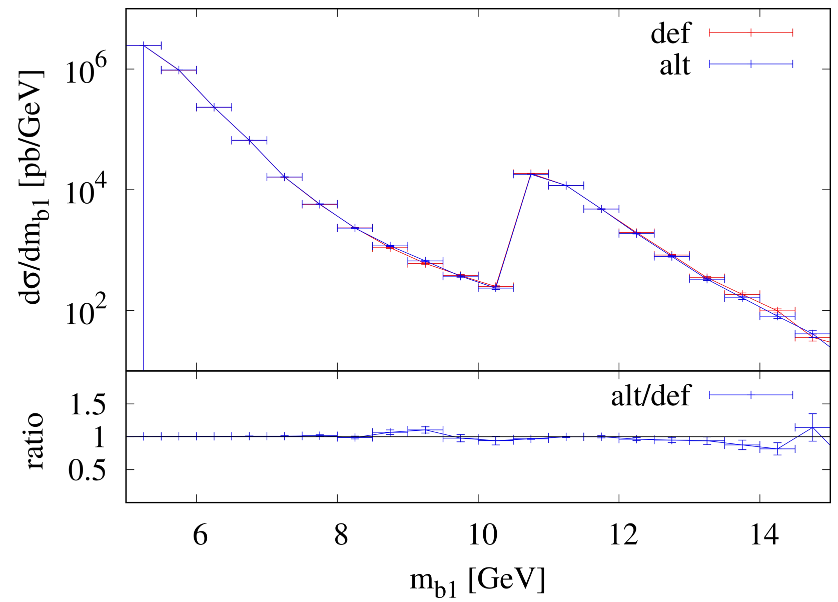
- **Observables of interest**: $p_{T,B}$ (transverse momentum of the b quark/hadron), mass and *profile* of the leading bjet

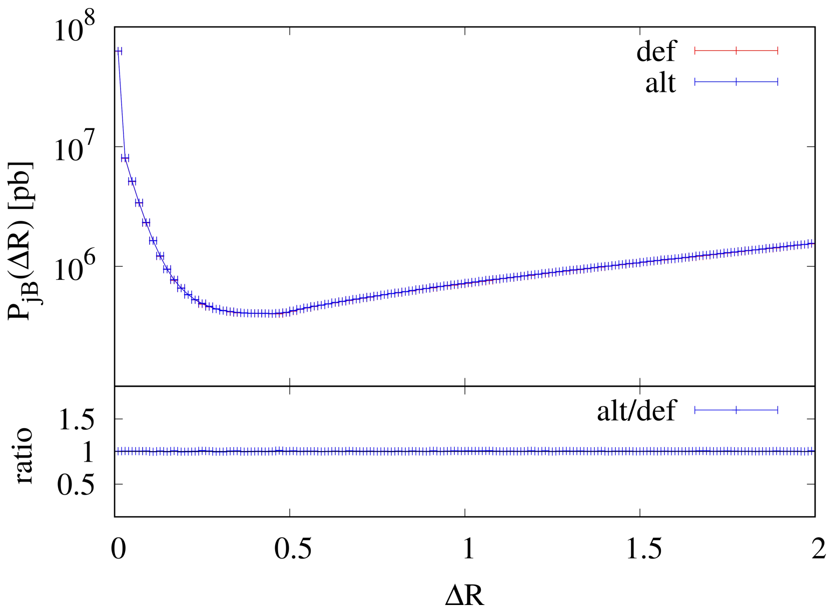
profile definition:

$$P_{j_b}(\Delta R) = \sum_j d\sigma \frac{p_T^j}{p_T^{j_b}} \delta(\Delta R - \Delta R^{j,j_b})$$

Preliminary Results - HVQ 200 GeV + PYTHIA8

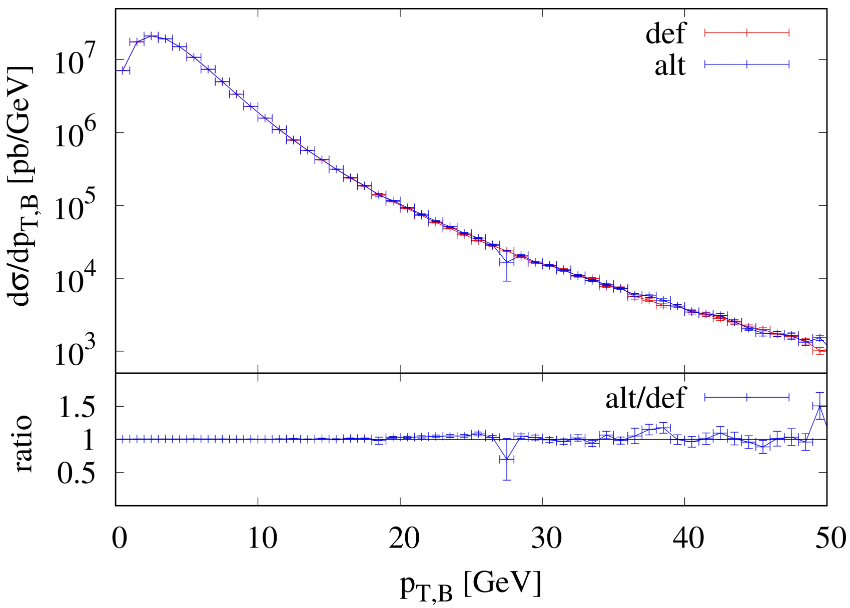


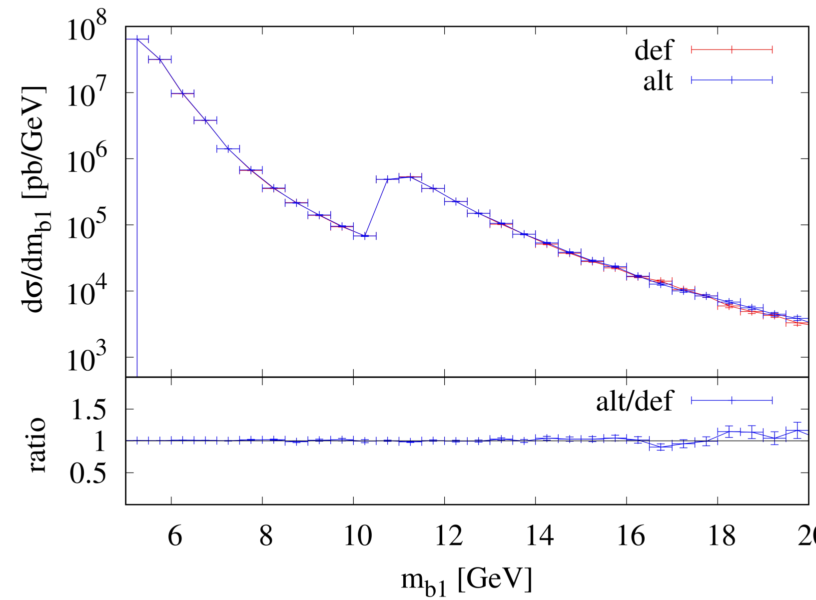


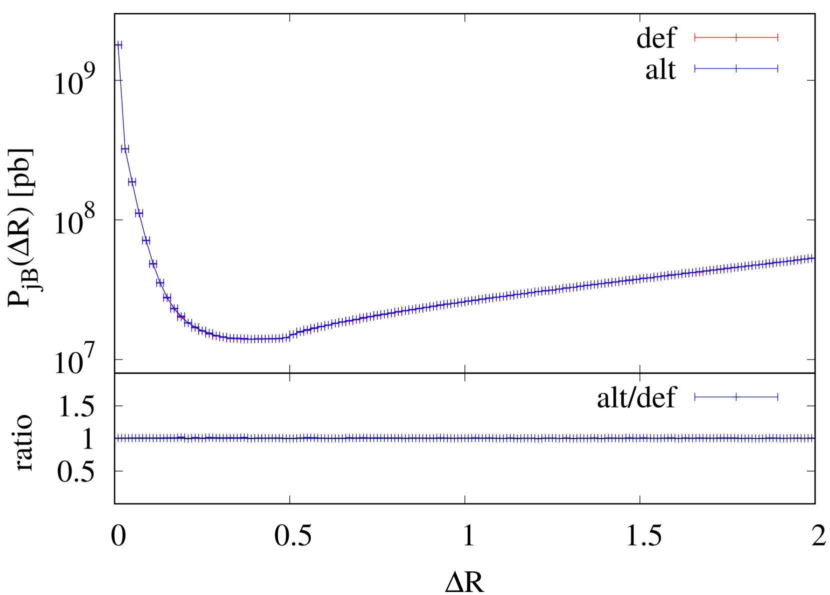


- Events generated: 500K/process
- **Wall Time:** 7h def
  2h alt
- Perfect aggreement between the two implementations

Preliminary Results - HVQ 1.96TeV + PYTHIA8

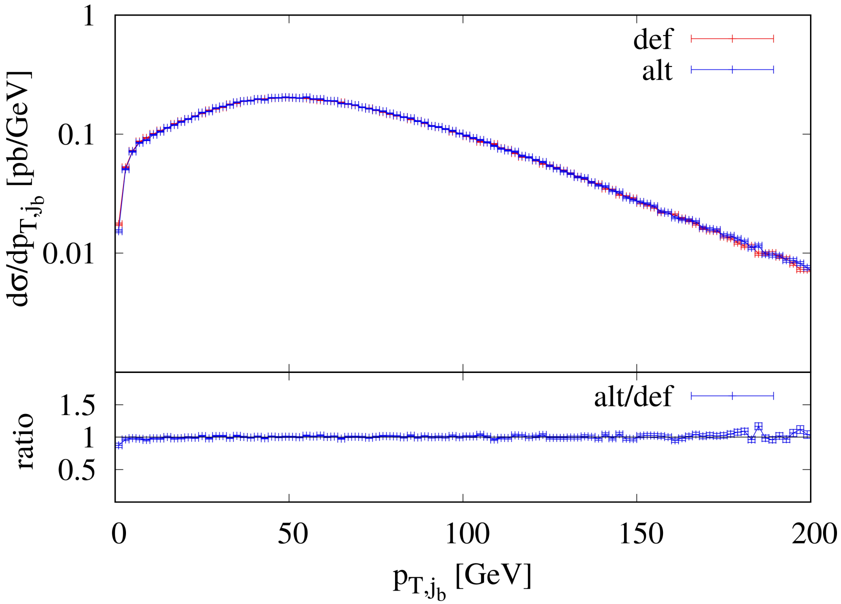


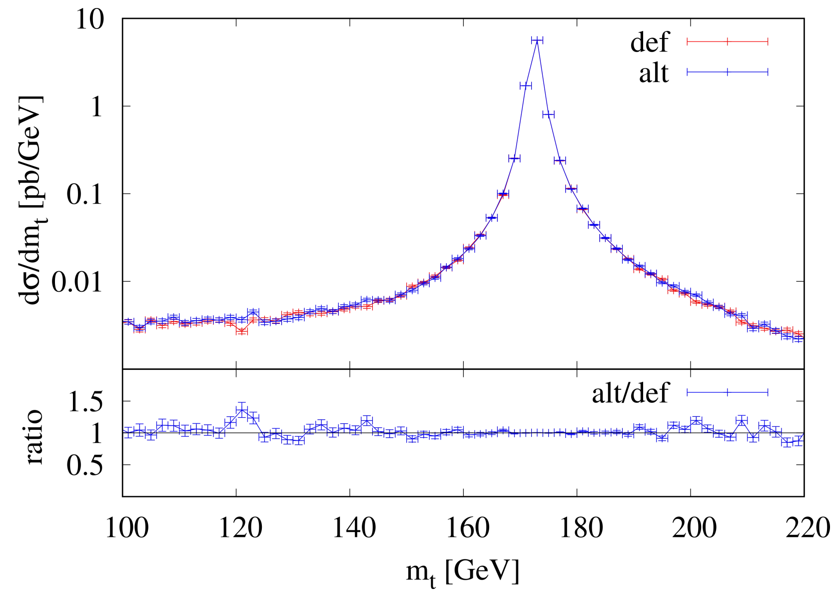


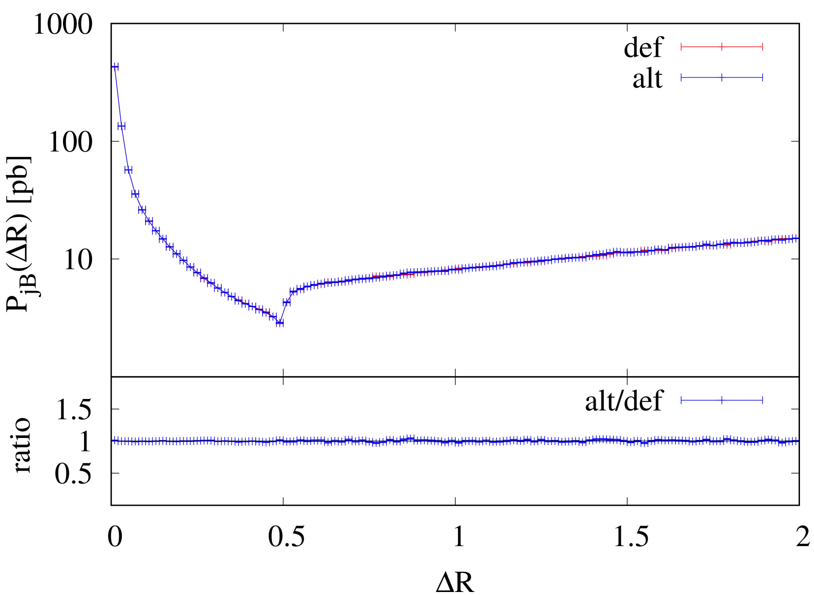


- Events generated: 500K/process
- **Wall Time:** 21h 30m def
  12h 24m alt
- Perfect aggreement between the two implementations

Preliminary Results - b_bar_4l 13TeV + PYTHIA8

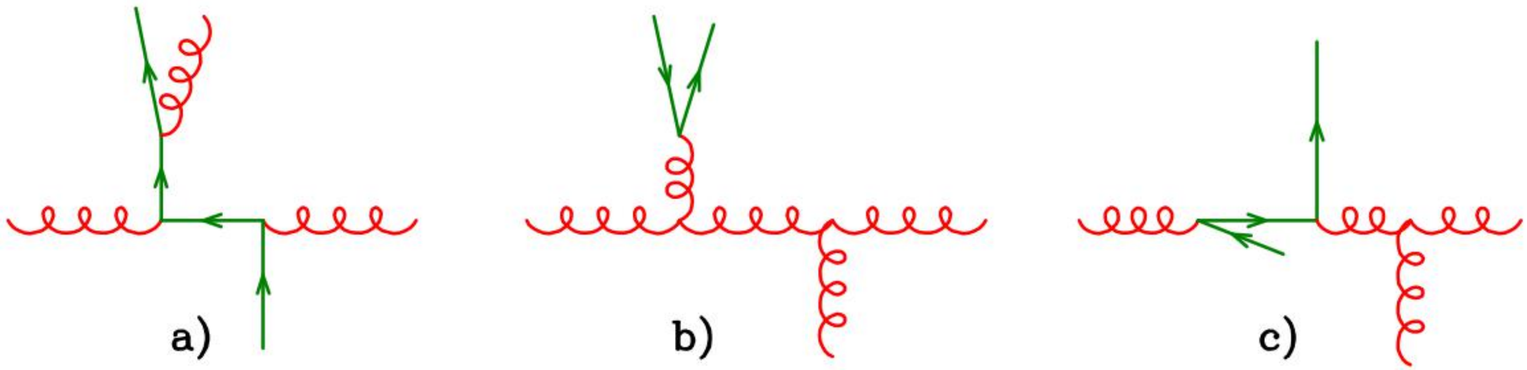






- Events generated: 21K/process
- **Wall Time:** 15h def
  7h 26m alt
- Perfect aggreement between the two implementations

Work in progress - "HVQ laboratory"



- Traditional HVQ (heavy quark as heavy) is supposed to give resonable results when the transverse momentum of the heavy quark is not too large.
- When the real kinematics is near to one of the enhanced region, the gluon transverse momentum is not small. **The numerator R may be enhanced with respect to the denominator B yelding a suppression of the real cross section** which is not justified.
- The **remnant mechanism** can be used to separate the three enhanced regions from the soft singular contribution.

$$D = \frac{d_{\mathrm{ISR}}^{-1}}{d_{\mathrm{ISR}}^{-1} + d_{\mathrm{glsp}}^{-1} + d_q^{-1} + d_{\bar{q}}^{-1} + d_{1q}^{-1} + d_{2q}^{-1} + d_{1\bar{q}}^{-1} + d_{2\bar{q}}}$$

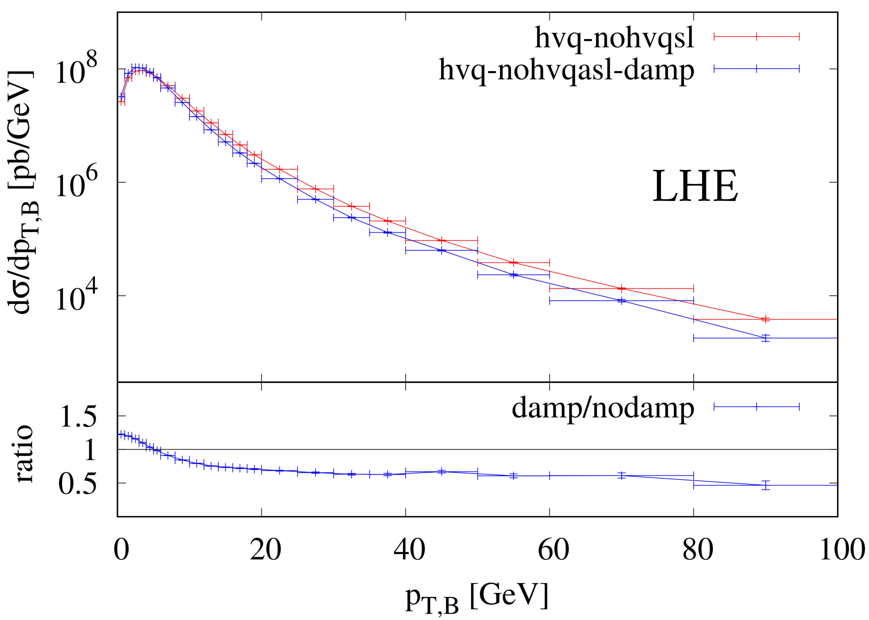
$$R = \mathrm{DR} + (1 - D)\, R = R_s + R_f$$

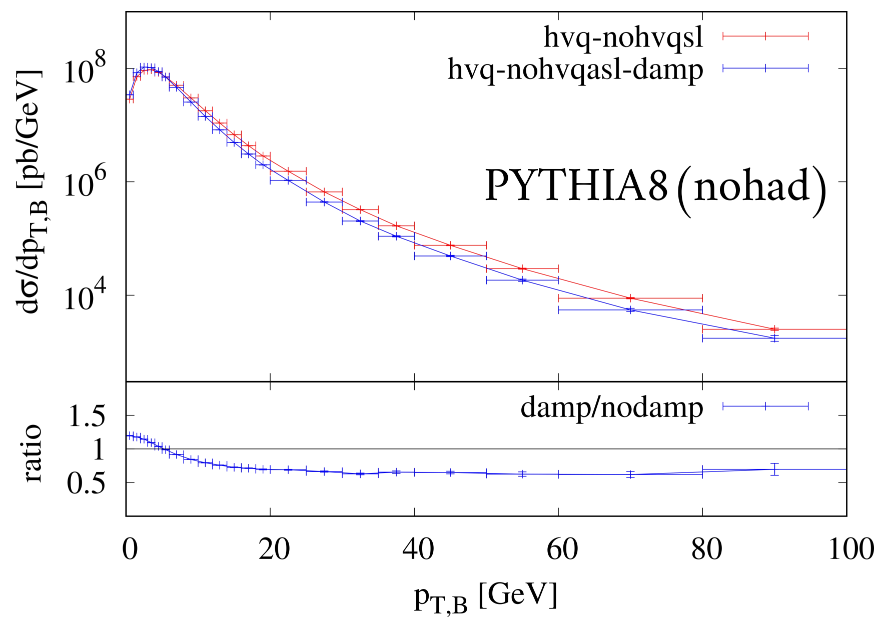
Work in progress - very preliminary

- When the **hvqaslight option** is enabled, heavy quark radiation regions are treated consistently as singular FSR regions. We must not separate them into the remnants:

$$D = \frac{d_{\rm ISR}^{-1} + d_q^{-1} + d_{\bar{q}}}{d_{\rm ISR}^{-1} + d_{\rm glsp}^{-1} + d_q^{-1} + d_{\bar{q}}^{-1} + d_{1q}^{-1} + d_{2q}^{-1} + d_{1\bar{q}}^{-1} + d_{2\bar{q}}} \qquad R_s^i = {\rm DR}^i, \quad R_f^i = {\rm DR}^i$$

- In standard POWHEG, remnants share the same scale choice as the Btilde contribution, which is of the order of the heavy quark transverse momentum in the underlying Born. This may lead to an underestimate of the scale and **it may be desiderable to have the scale in the remnant evaluating according to the real emission kinematics**.





Summary and conclusions

- Radiation from heavy quarks may have a relevant impact on hot topics in LHC physics.
- A new phase space mapping for massive fermions has been proposed based on a solid physical background.
- A full and well tested implementation has been given in POWHEG-BOX-RES which has proven superior to the previous one in terms of computational efficiency.
- A deeper understanding of heavy flavour dynamics may come from HVQ generator analysis. Phenomenological studies are just beginning, stay tuned!