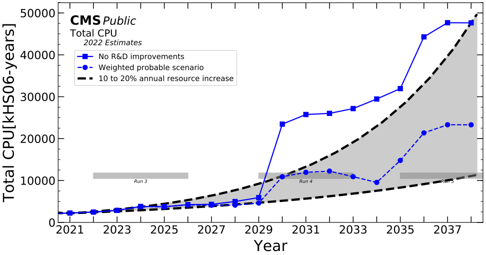
Forced heavy flavour hadronisation in Pythia

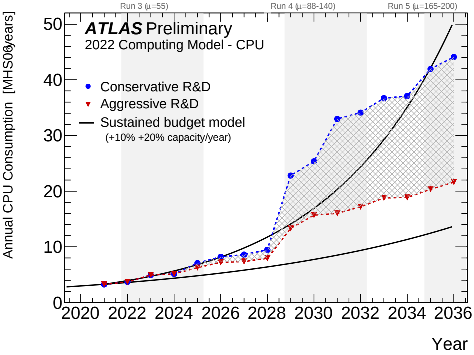
A method to speed up simulation of rare heavy flavour processes

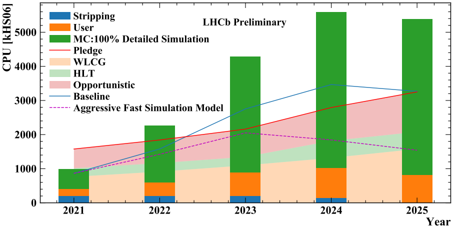
Riley Henderson, Peter Skands

MONASH University

LHC computing projections







Aggressive R&D needed!

Without it, CPU needs will quickly become unmanageable with current expected budgets.

Simulation of rare heavy flavour processes

MONASH University

- For LHCb in particular, part of the problem stems from the rarity of the processes being simulated.
- This makes the *generation* of events slow, which is becoming an increasingly significant portion of the total simulation time.
  - Note: simulation of the detector and event reconstruction is usually dominant — but this is a topic for another day.
- Slow event generation is a compound effect from several sources:
  1. Heavy flavour production rates in inclusive samples, *e.g.* $\sigma(pp \to b\bar{b}X)$.
  2. Heavy flavour hadron production fractions, *e.g.* $\mathcal{B}(b \to H_b)$.
  3. Phase space cuts or any other extra requirements imposed.

Type(s) of b hadron:	B^0, B^+	B_s^0, Λ_b^0	Υ, Ξ_b	Σ_b, B_c^+	Ω_b^-, Ξ_{bc}
Rate in inclusive sample:	$\mathcal{O}(10^{-2})$	$\mathcal{O}(10^{-3})$	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{-5})$	$\leq \mathcal{O}(10^{-6})$

Simulation of rare heavy flavour processes

- For LHCb in particular, part of the problem stems from the rarity of the processes being simulated.
- This makes the *generation* of events slow, which is becoming an increasingly significant portion of the total simulation time.
  - Note: simulation of the detector and event reconstruction is usually dominant — but this is a topic for another day.
- Slow event generation is a compound effect from several sources:
  1. Heavy flavour production rates in inclusive samples, *e.g.* $\sigma(pp \to b\bar{b}X)$.
  2. Heavy flavour hadron production fractions, *e.g.* $\mathcal{B}(b \to H_b)$.
  3. Phase space cuts or any other extra requirements imposed.
- Large differences in rates for b-hadrons caused by the different production fractions.

Type(s) of b hadron:	B^0, B^+	B_s^0, Λ_b^0	Υ, Ξ_b	Σ_b, B_c^+	Ω_b^-, Ξ_{bc}
Rate in inclusive sample:	$\mathcal{O}(10^{-2})$	$\mathcal{O}(10^{-3})$	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{-5})$	$\leq \mathcal{O}(10^{-6})$

Simulation of rare heavy flavour processes

- For LHCb in particular, part of the problem stems from the rarity of the processes being simulated.
- This makes the *generation* of events slow, which is becoming an increasingly significant portion of the total simulation time.
  - Note: simulation of the detector and event reconstruction is usually dominant — but this is a topic for another day.
- Slow event generation is a compound effect from several sources:
  1. Heavy flavour production rates in inclusive samples, *e.g.* $\sigma(pp \to b\bar{b}X)$.
  2. Heavy flavour hadron production fractions, *e.g.* $\mathcal{B}(b \to H_b)$.
  3. Phase space cuts or any other extra requirements imposed.
- Large differences in rates for b-hadrons caused by the different production fractions.

Type(s) of b hadron:	B^0, B^+	B^0_s, Λ^0_b	Υ, Ξ_b	Σ_b, B^+_c	Ω^-_b, Ξ_{bc}
Rate in inclusive sample:	$\mathcal{O}(10^{-2})$	$\mathcal{O}(10^{-3})$	$\mathcal{O}(10^{-4})$	$\mathcal{O}(10^{-5})$	$\leq \mathcal{O}(10^{-6})$

- **Wouldn't it be nice if we could simulate rare b-hadrons just as quickly as common ones...**

Heavy flavour hadron production

- The main production mechanisms for most of these *b*-hadrons are:
  1. **Fragmentation**: heavy quarks combine with new flavours produced out of the vacuum to form hadrons.
  2. **Decays**: lighter hadrons can result from decays of heavier hadrons produced earlier, *e.g.* by fragmentation.
- In general, production of $q\bar{q}$ pairs in the *fragmentation* is strongly suppressed by quark masses, making heavy hadrons rare and thus slow to generate.

Heavy flavour hadron production

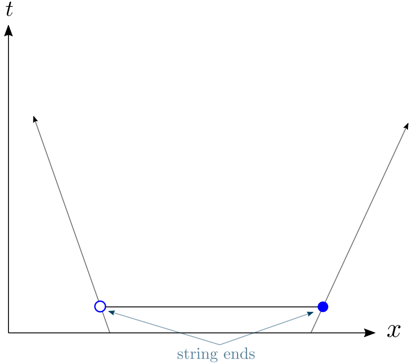
- The main production mechanisms for most of these b-hadrons are:
  1. **Fragmentation**: heavy quarks combine with new flavours produced out of the vacuum to form hadrons.
  2. **Decays**: lighter hadrons can result from decays of heavier hadrons produced earlier, *e.g.* by fragmentation.
- In general, production of $q\bar{q}$ pairs in the *fragmentation* is strongly suppressed by quark masses, making heavy hadrons rare and thus slow to generate.
- In the Pythia fragmentation algorithm:
  - Strange ($s\bar{s}$) suppressed by a factor $\sim \frac{1}{10}$ relative to $u\bar{u}$ or $d\bar{d}$.
  - Baryons (via $qq'\overline{qq}'$) suppressed by a factor $\sim \frac{1}{13}$ relative to mesons.
  - The above two suppression factors effects are compounded for strange baryons.
  - Charm or heavier suppressed by a factor $\leq 10^{-11}$ (assumed zero in Pythia, *i.e.* cannot happen).

Heavy flavour hadron production

- The main production mechanisms for most of these b-hadrons are:
  1. **Fragmentation**: heavy quarks combine with new flavours produced out of the vacuum to form hadrons.
  2. **Decays**: lighter hadrons can result from decays of heavier hadrons produced earlier, *e.g.* by fragmentation.
- In general, production of $q\bar{q}$ pairs in the *fragmentation* is strongly suppressed by quark masses, making heavy hadrons rare and thus slow to generate.
- In the Pythia fragmentation algorithm:
  - Strange ($s\bar{s}$) suppressed by a factor $\sim \frac{1}{10}$ relative to $u\bar{u}$ or $d\bar{d}$.
  - Baryons (via $qq'\overline{qq}'$) suppressed by a factor $\sim \frac{1}{13}$ relative to mesons.
  - The above two suppression factors effects are compounded for strange baryons.
  - Charm or heavier suppressed by a factor $\leq 10^{-11}$ (assumed zero in Pythia, *i.e.* cannot happen).
- **In principle, it is possible to effectively remove some of these suppression factors in the Pythia fragmentation algorithm... provided the relative probabilities are accounted for with event weights.**
- This should bring $\sim$ 10x or more improvements in efficiency for rare hadrons.

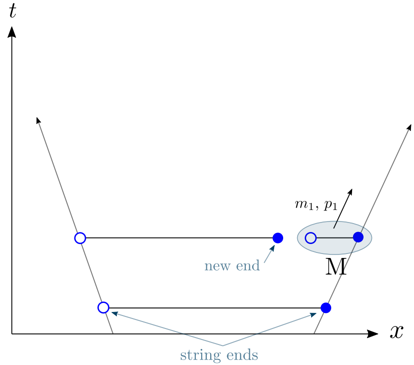
Pythia hadronisation model

- The formation of hadrons in Pythia is based on the **Lund string model**.
- Partons produced eariler in the event are connected by strings representing QCD colour confining strong interactions.
- Strings then *fragment* into hadrons via the creation of quark-antiquark pairs along the string, causing it to break up.



Pythia hadronisation model

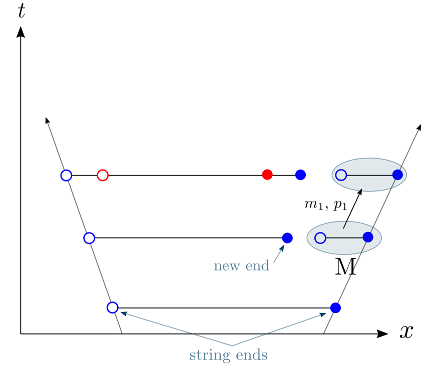
- The formation of hadrons in Pythia is based on the **Lund string model**.
- Partons produced eariler in the event are connected by strings representing QCD colour confining strong interactions.
- Strings then *fragment* into hadrons via the creation of quark-antiquark pairs along the string, causing it to break up.



- Mesons can be produced from the creation of a single quark-antiquark pair.

Pythia hadronisation model

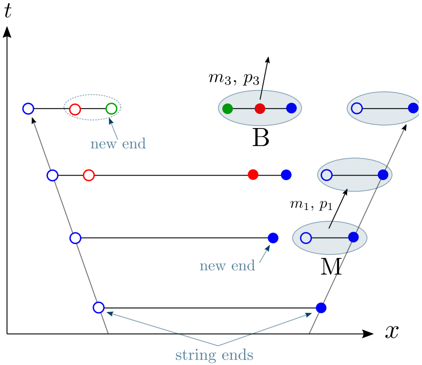
- The formation of hadrons in Pythia is based on the **Lund string model**.
- Partons produced eariler in the event are connected by strings representing QCD colour confining strong interactions.
- Strings then *fragment* into hadrons via the creation of quark-antiquark pairs along the string, causing it to break up.



- Mesons can be produced from the creation of a single quark-antiquark pair.
- Baryons require the creation of a diquark-antidiquark pair.
  1. Modelled as successive creation of quark-antiquark pairs.

Pythia hadronisation model

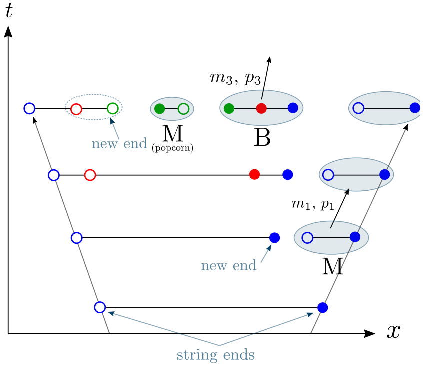
- The formation of hadrons in Pythia is based on the **Lund string model**.
- Partons produced eariler in the event are connected by strings representing QCD colour confining strong interactions.
- Strings then *fragment* into hadrons via the creation of quark-antiquark pairs along the string, causing it to break up.



- Mesons can be produced from the creation of a single quark-antiquark pair.
- Baryons require the creation of a diquark-antidiquark pair.
  1. Modelled as successive creation of quark-antiquark pairs.

Pythia hadronisation model

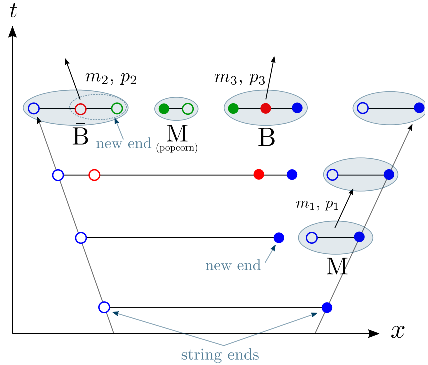
- The formation of hadrons in Pythia is based on the **Lund string model**.
- Partons produced eariler in the event are connected by strings representing QCD colour confining strong interactions.
- Strings then *fragment* into hadrons via the creation of quark-antiquark pairs along the string, causing it to break up.



- Mesons can be produced from the creation of a single quark-antiquark pair.
- Baryons require the creation of a diquark-antidiquark pair.
  1. Modelled as successive creation of quark-antiquark pairs.
  2. Can also produce additional "popcorn" mesons between the baryons.

Pythia hadronisation model

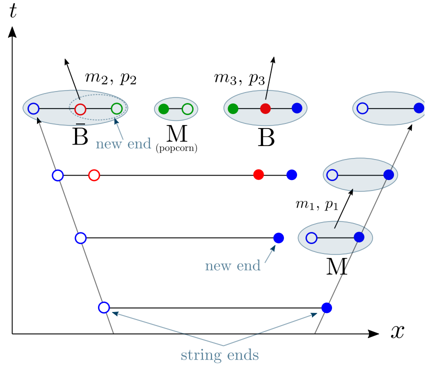
- The formation of hadrons in Pythia is based on the **Lund string model**.
- Partons produced eariler in the event are connected by strings representing QCD colour confining strong interactions.
- Strings then *fragment* into hadrons via the creation of quark-antiquark pairs along the string, causing it to break up.



- Mesons can be produced from the creation of a single quark-antiquark pair.
- Baryons require the creation of a diquark-antidiquark pair.
  1. Modelled as successive creation of quark-antiquark pairs.
  2. Can also produce additional "popcorn" mesons between the baryons.

Pythia hadronisation model

- The formation of hadrons in Pythia is based on the **Lund string model**.
- Partons produced eariler in the event are connected by strings representing QCD colour confining strong interactions.
- Strings then *fragment* into hadrons via the creation of quark-antiquark pairs along the string, causing it to break up.

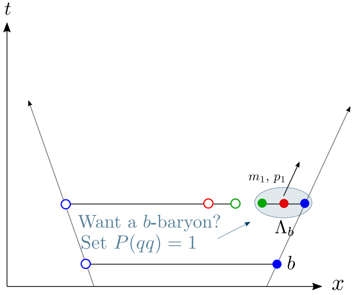


- Mesons can be produced from the creation of a single quark-antiquark pair.
- Baryons require the creation of a diquark-antidiquark pair.
  1. Modelled as successive creation of quark-antiquark pairs.
  2. Can also produce additional "popcorn" mesons between the baryons.
- Different flavoured hadrons can be produced depending on the (random) flavour of the new quarks.
- **Heavy quarks can only be string endpoints.**

- Flavour selection probabilities can be biased in the fragmentation algorithm to force specific *b*-hadrons to appear.

Example: force *b*-baryon

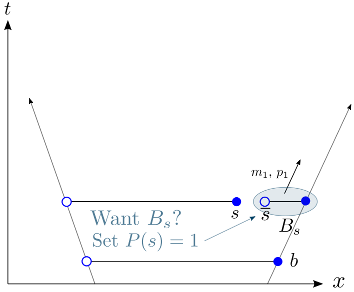
Set diquark probability to 1.



Example: force B_s^0

Set diquark probability to zero.

Set strange quark probability to 1.



Pretty straightforward. But... which *b* quarks should be forced? And into which hadrons? What should the event weight be? etc.

Forcing method

1. Randomly select one b (or $\overline{b}$) quark in the event to have its fragmentation biased.
2. Choose a (class of) b-hadron(s) H_b to force. For now, we have looked at:
   - Strange beauty hadrons.
   - Beauty baryons.
   - Strange beauty baryons.
   - Could also choose to force specific individual hadrons.
3. Manipulate flavour selection to guarantee the “forced type” hadron, *i.e.* $P(H_b) \rightarrow 1$.
4. Calculate an event weight based on the probability of obtaining the forced type hadron H_b in an *unbiased* sample.

Forcing method

1. Randomly select one b (or $\overline{b}$) quark in the event to have its fragmentation biased.
2. Choose a (class of) b-hadron(s) H_b to force. For now, we have looked at:
   - Strange beauty hadrons.
   - Beauty baryons.
   - Strange beauty baryons.
   - Could also choose to force specific individual hadrons.
3. Manipulate flavour selection to guarantee the "forced type" hadron, *i.e.* $P(H_b) \to 1$.
4. Calculate an event weight based on the probability of obtaining the forced type hadron H_b in an *unbiased* sample.

- The bulk of the work to implement this correctly is evidently in the calculation of the event weights.
- The current status is that we have not quite nailed this down perfectly yet :(
- I will go through the main details and show our progress + some discoveries we've made.

Event weight

The event weight is defined such that the probability of obtaining the forced type hadron in an unbiased sample is reproduced:

- Let n_b denote the number of forcing candidates (b quarks), in an event.
- Let n_s be the number of forced type hadrons produced in the event.
- Let $P(H_b)$ be the unbiased probability to obtain the forced type hadron from a single b quark.
- Forcing implies $P(H_b \to 1)$, and the appropriate event should be given by

$$w = \frac{n_b}{n_s} P(H_b). \tag{1}$$

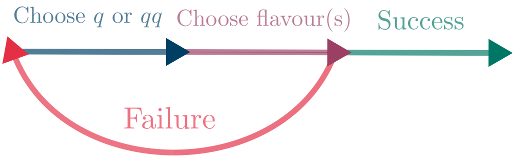
- **The most important thing to calculate is the unbiased probability $P(H_b)$ of obtaining the forced type hadron.**

Hadron probabilities

- The probability to *select* a given b-hadron flavour is fully determined by a set of fixed input parameters.
- The main ones are:
  1. $P(s)/P(u|d) = 0.217$: single strange suppression relative to up/down.
  2. $P(qq)/P(q) = 0.081$: diquark suppression relative to single quarks.
  3. Diquarks with strange content have more complicated conditional probabilities (but still constant).
- The only problem is that flavour selection is not the only factor in the final b-hadron probability...

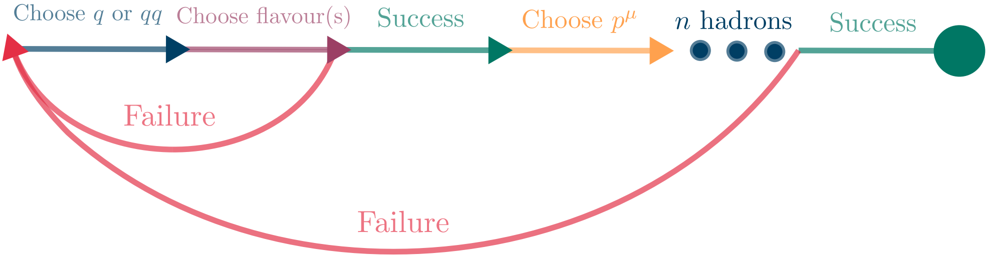
Rejection loops in the fragmentation

1. There are points in the Pythia string fragmentation algorithm where a particular flavour selection can be rejected.
   - In these cases, new flavour selections are repeatedly tried until one succeeds.



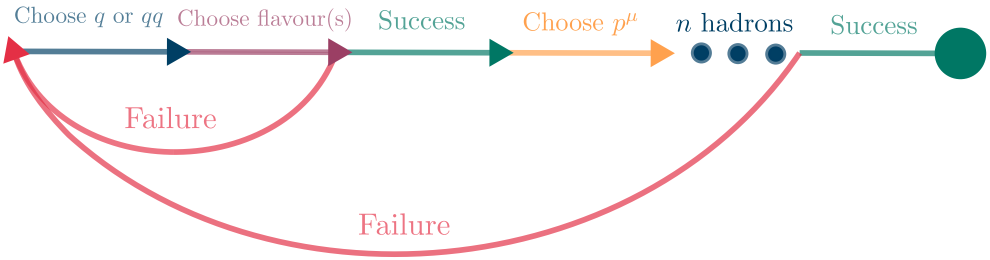
Rejection loops in the fragmentation

1. There are points in the Pythia string fragmentation algorithm where a particular flavour selection can be rejected.
   - In these cases, new flavour selections are repeatedly tried until one succeeds.
2. The string fragmentation algorithm in Pythia is not guaranteed to produce a physical hadron configuration.
   - In these cases, the hadrons are discarded and the entire string is refragmented from the start.



Rejection loops in the fragmentation

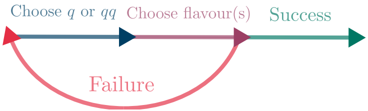
1. There are points in the Pythia string fragmentation algorithm where a particular flavour selection can be rejected.
   - In these cases, new flavour selections are repeatedly tried until one succeeds.
2. The string fragmentation algorithm in Pythia is not guaranteed to produce a physical hadron configuration.
   - In these cases, the hadrons are discarded and the entire string is refragmented from the start.



This means that for any hadron produced in the fragmentation, there may have been an arbitrary number of failures prior to its success.

Hadron (baryon) rejection loop

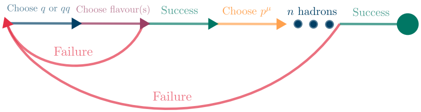
- The possibility of randomly rejecting a flavour selection leads to the *hadron rejection loop*.
- In fact, only diquark selections can fail by default, therefore it is really a *baryon rejection loop*.
  - Any successful hadron may have been preceded by an arbitrary number of failed baryons.



- The probability for a baryon to be rejected depends on a small set of fixed survival probabilities.
- The contribution to the final b-hadron probabilities is universal and can therefore be calculated in a straightforward manner.

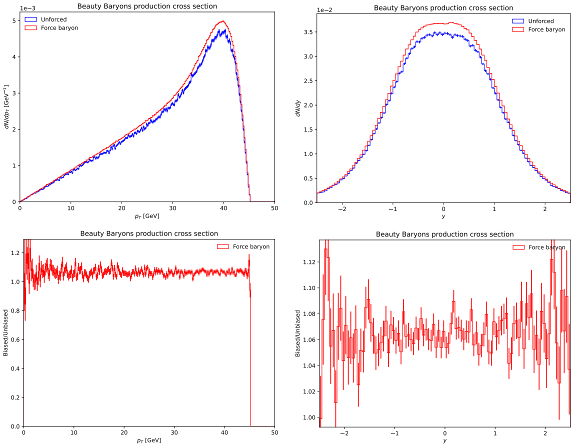
String rejection loop

- The string rejection loop is not so straightforward.
- The success/failure probability depends on the string energy, and potentially other hadrons produced on the string.



- Evidently, this effect is not negligible and results in 5–10% discrepancies between biased/unbiased distributions.
- I am currently working on finding a solution to this issue.
- Analytical calculation might be possible seems quite difficult.
- Currently focussing on more empirical approaches to find an appropriate weighting method.
- For now, I have only partial results that are not quite weighted correctly.

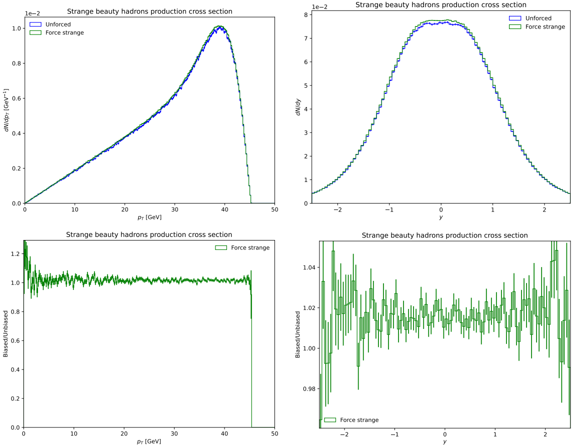
Example 1: Forced *b*-baryons



- Set diquark probability $P(qq) \to P'(qq) = 1$ for the forced b quark, guaranteeing a baryon is always selected.
- Event weight determined by the unbiased probability to obtain any b-baryon.
- Event weight currently not considering string rejection loop.
  - Biased/unbiased ≈ 1.06.

Plots show (left) p_{T} and (right) y spectrum for all baryons. Bottom plots are the ratio biased/unbiased.

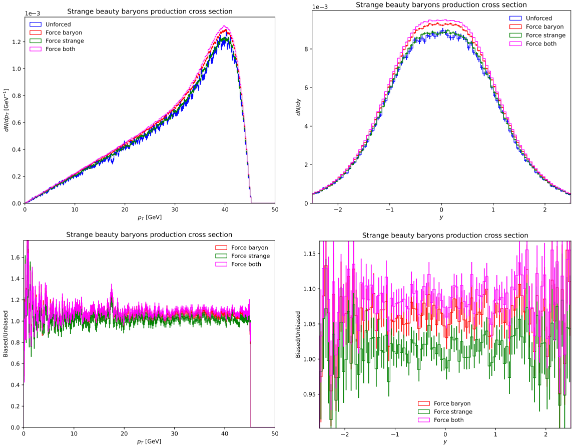
Example 2: Force strange hadrons



- Bias strange quark selection probabilities for the forced b quark to guarantee at least one unit of strangeness.
- Event weight determined by the total unbiased probability to obtain a b-hadron.
- Event weight currently not considering string rejection loop.
  - Biased/unbiased ≈ 1.02.

Plots show (left) p_T and (right) y spectrum for all baryons.
Bottom plots are the ratio biased/unbiased.

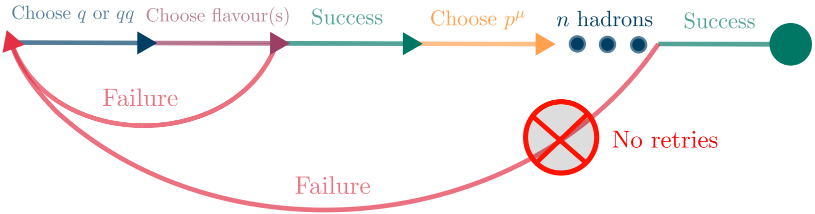
Example 3: Force strange b-baryons



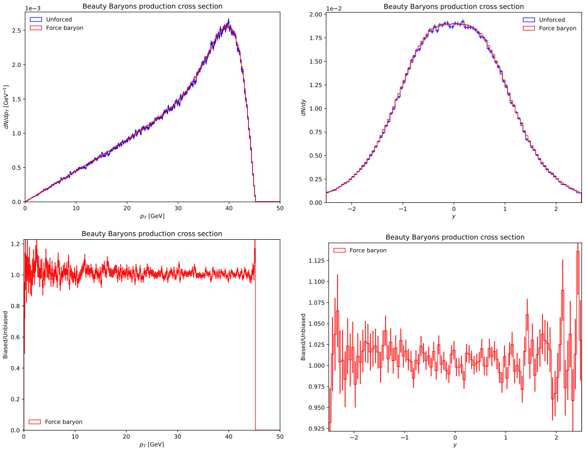
- Set diquark probability $P(qq) \to P'(qq) = 1$ AND bias strange quark selection probabilities for the forced b quark to guarantee at least one unit of strangeness.
- Event weight determined by the unbiased probability to obtain any strange b-baryon.
- Event weight currently not considering string rejection loop.
  - Biased/unbiased ≈ 1.09. for forcing strange baryons.

Plots show (left) p_{T} and (right) y spectrum for all baryons. Bottom plots are the ratio biased/unbiased.

- Evidently, the string rejection loop is almost entirely responsible for the remaining disagreement between biased and unbiased samples.
- To see this, consider only the events in which the forced b string fragments successfully on the first try.
- The string rejection loop therefore does not contribute to the probability for these events and can be neglected in the event weight.

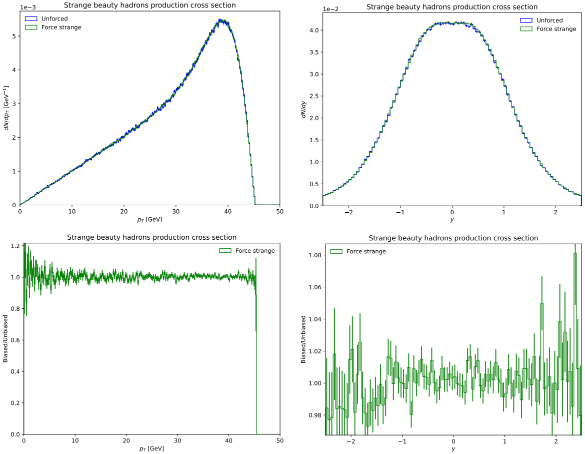


Example 1: Force b-baryons



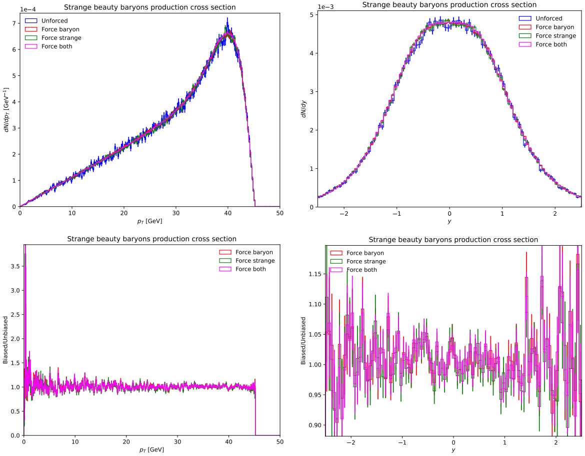
Plots show (left) p_{T} and (right) y spectrum for all baryons.

Example 3: Forced strange b-hadrons



Plots show (left) p_{T} and (right) y spectrum for strange baryons.

Example 3: Force strange b-baryons



Plots show (left) p_T and (right) y spectrum for strange baryons.

Summary

- I have implemented options in Pythia to force the presence of specific rare heavy flavour hadrons in events that contain a heavy flavour quark.
- This should bring $\sim$ 10x improvements in the efficiency of generating rare heavy flavour hadrons.
- Calculation of the appropriate event weights is almost there but still ongoing.
- Currently, the weights are off by 5–10% due to the possibility of strings being refragmented many times.
- Still working on a solution to this problem.

Thanks for listening.

Backup

Conditional diquark probabilities

- Diquarks composed of a “popcorn” quark q_p and a “vertex” quark q_v.
- The probability to select a given flavour for the vertex quark depends upon the flavour of the popcorn quark — specifically, whether or not it is strange.
- For a nonstrange diquark with flavour content qq', the relevant unbiased probabilities are,

$$\begin{aligned} P(q_p \,\&\, q'_v) &= P(q_p)P(q'_v|!s_p), \\ P(q'_p \,\&\, q_v) &= P(q'_p)P(q_v|!s_p), \end{aligned} \tag{2}$$

while for a singly strange diquark sq, the relevant probabilities are

$$\begin{aligned} P(s_p \,\&\, q_v) &= P(s_p)P(q_v|s_p), \\ P(q_p \,\&\, s_v) &= P(q_p)P(s_v|!s_p), \end{aligned} \tag{3}$$

and for a doubly strange diquark,

$$P(s_p \,\&\, s_v) = P(s_p)P(s_v|s_p), \tag{4}$$

Event weight

The event weight is defined such that the probability of obtaining the forced type hadron in an unbiased sample is reproduced:

- Let n_b denote the number of forcing candidates (b quarks), in an event.
- Let n_s be the number of "forced type" hadrons produced in the event.
- Unbiased probability to obtain n_s forced type hadrons is a binomial distribution:

$$P(n_s, n_b, P_s) = \binom{n_b}{n_s} P_s^{n_s} (1 - P_s)^{n_b - n_s} , \tag{5}$$

  where $P_s \equiv P(H_b)$ is the unbiased probability to obtain the forced type hadron through fragmentation of one parton.
- Biasing the probability of obtaining the forced type hadron amounts to changing $P_s \to P_s'$ for only the chosen b quark.
- *Biased* probability to obtain n_s forced type hadrons is now given by:

$$P'(n_s, n_b, P_s, P_s') = \left[\frac{P_s'}{P_s} \frac{n_s}{n_b} + \frac{n_b - n_s}{n_b} \frac{(1 - P_s')}{(1 - P_s)} \right] P(n_s, n_b, P_s). \tag{6}$$

- Apply event weight w to the biased events such that,

$$wP'(n_s, n_b, P_s, P'_s) = P(n_s, n_b, P_s), \tag{7}$$

- The event weight is then given by

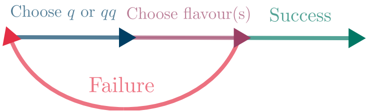
$$w = \frac{P(n_s, n_b, P_s)}{P'(n_s, n_b, P_s, P'_s)} = \left[\frac{P'_s}{P_s}\frac{n_s}{n_b} + \frac{n_b - n_s}{n_b}\frac{(1-P'_s)}{(1-P_s)}\right]^{-1}. \tag{8}$$

- If forcing guarantees the hadron, *i.e.* $P'_s = 1$, then the weight reduces to

$$w = \frac{n_b}{n_s} P_s. \tag{9}$$

- **The most important thing to calculate is the unbiased probability $P_s \equiv P(H_b)$ of obtaining the forced type hadron.**

Hadron (baryon) rejection loop



- The possibility of randomly rejecting a flavour selection leads to the *hadron rejection loop*.
- In fact, only diquark selections can fail by default, therefore it is really a *baryon rejection loop*.
  - Any successful hadron may have been preceded by an arbitrary number of failed baryons.
- The contribution to the overall hadron probabilities can be calculated straightforwardly.
- Let $P(f_k)$ and $P(S|f_k)$ be the selection and success probabilities for spin-flavour combination f_k, respectively. The probability that a baryon selection fails N times is then given by

$$P(\mathrm{F}_B, N) = P(\mathrm{F}_B, 1)^N = P(qq)^N \left[1 - \sum_k P(f_k) P(\mathrm{S}|f_k)\right]^N. \quad (10)$$

- The probability $P(h)$ for any hadron to succeed is then $P(h) = P_h P(\mathrm{F}_B)$, where

$$P(\mathrm{F}_B) = \sum_{i=0}^{\infty} P(\mathrm{F}_B, 1)^i = \frac{1}{1 - P(qq)\left[1 - \sum_k P(f_k) P(\mathrm{S}|f_k)\right]}, \quad (11)$$

and P_h is the probability to select hadron h in a single step.