Five-flavour scheme predictions for $t\bar{t}b\bar{b}$ at next-to-leading order accuracy in MG5_aMC@NLO

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based on:
R. Frederix, TM EPJC 84, 763 (2024)

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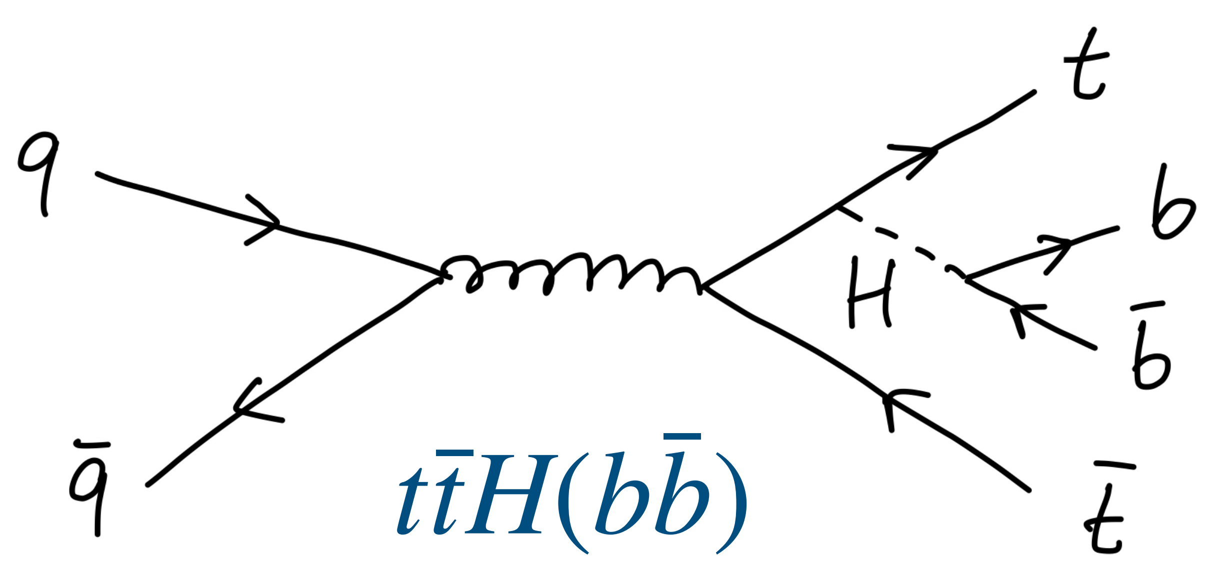
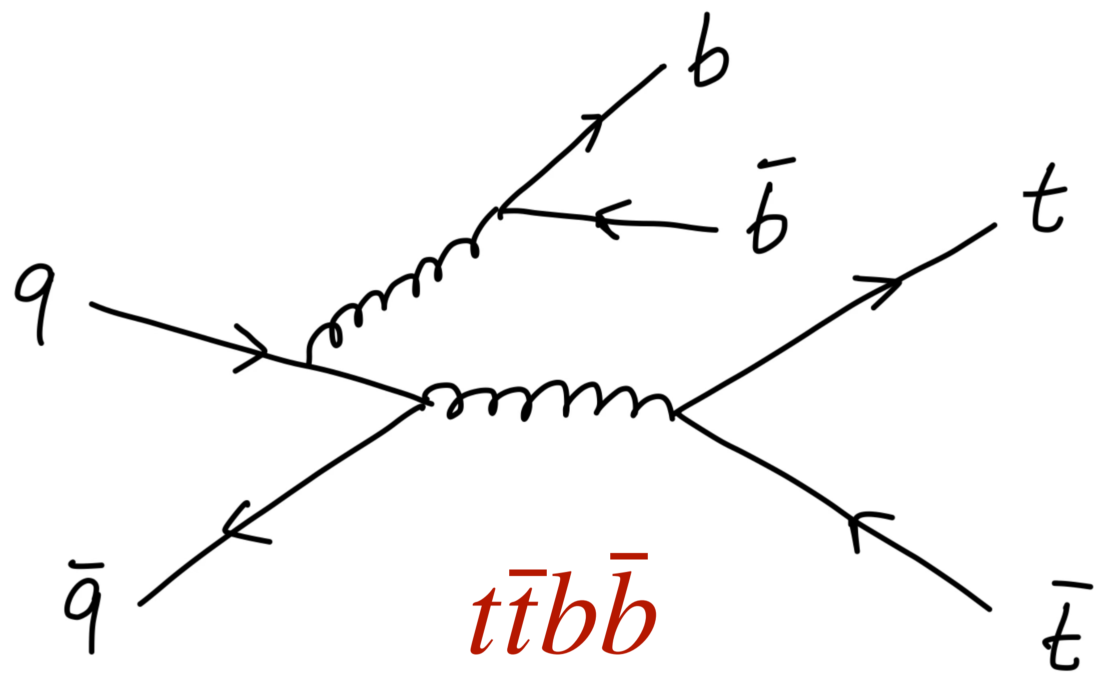
Role of the $t\bar{t}b\bar{b}$ process in the physics analyses

$t\bar{t}b\bar{b}$ represents a significant background in measurements probing the top Yukawa coupling

latest $t\bar{t}H(\to b\bar{b})$ from ATLAS PLB 849 (2024) and CMS arXiv:2407.10896

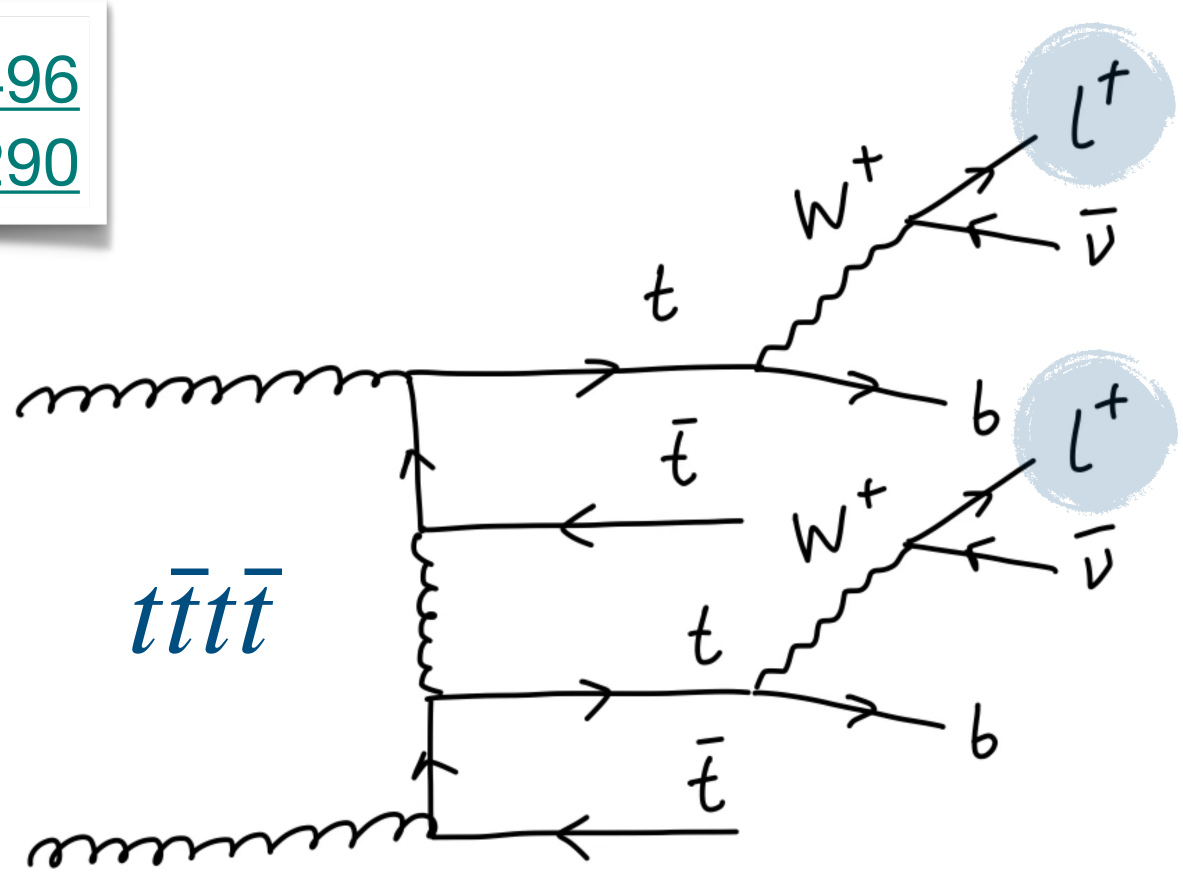
- $t\bar{t}H(\to b\bar{b})$ analyses
  - $t\bar{t}b\bar{b}$ is the dominant background
  - modelling uncertainty is currently a limitation

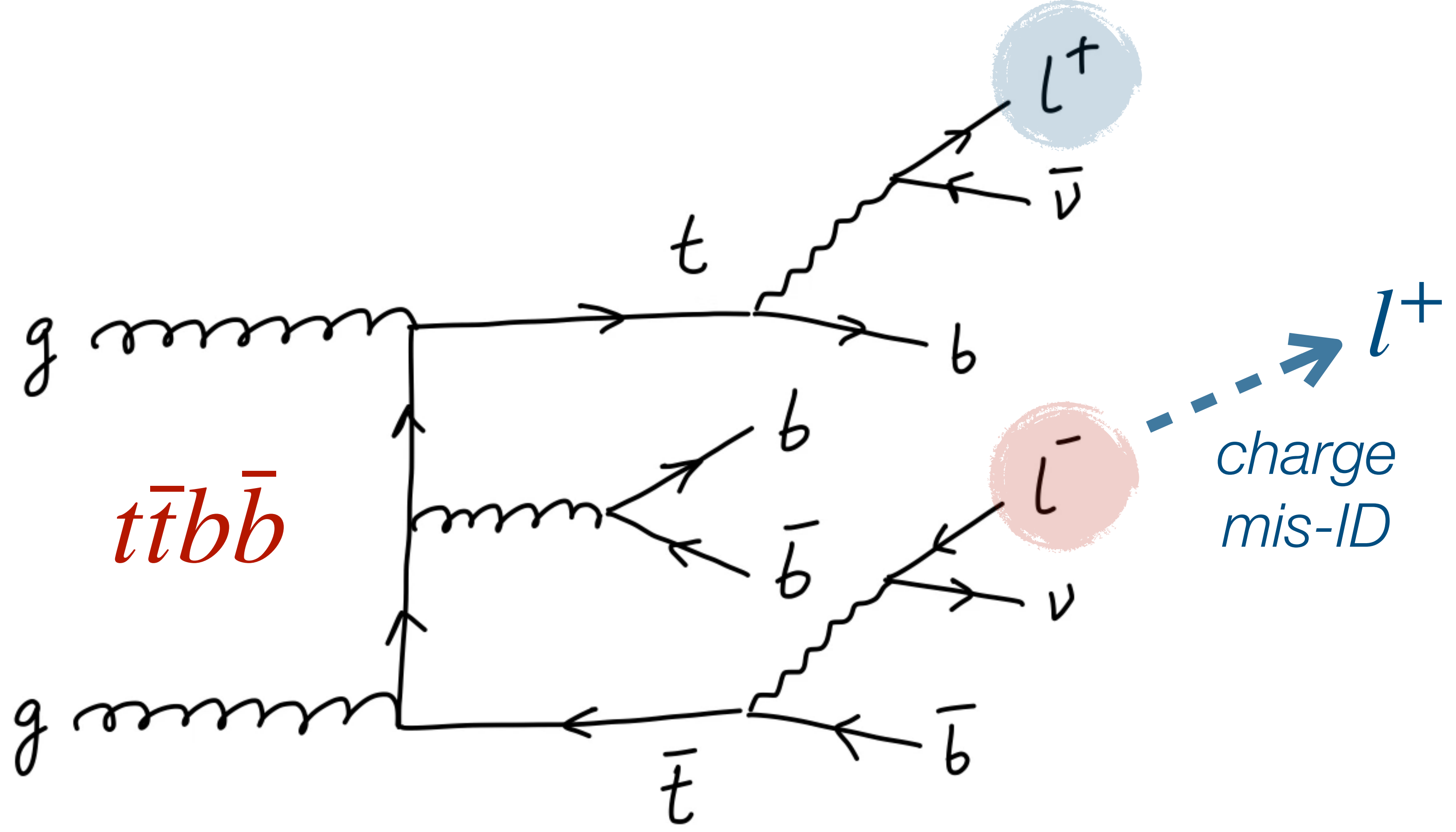




latest $t\bar{t}t\bar{t}$ from ATLAS EPJC 83 (2023) 6, 496 and CMS PLB 847 (2023) 138290

- 4-top analyses
  - $t\bar{t}$+jets (with additional b-jets) is the main source of fake/non-prompt and charge-mis-identification backgrounds



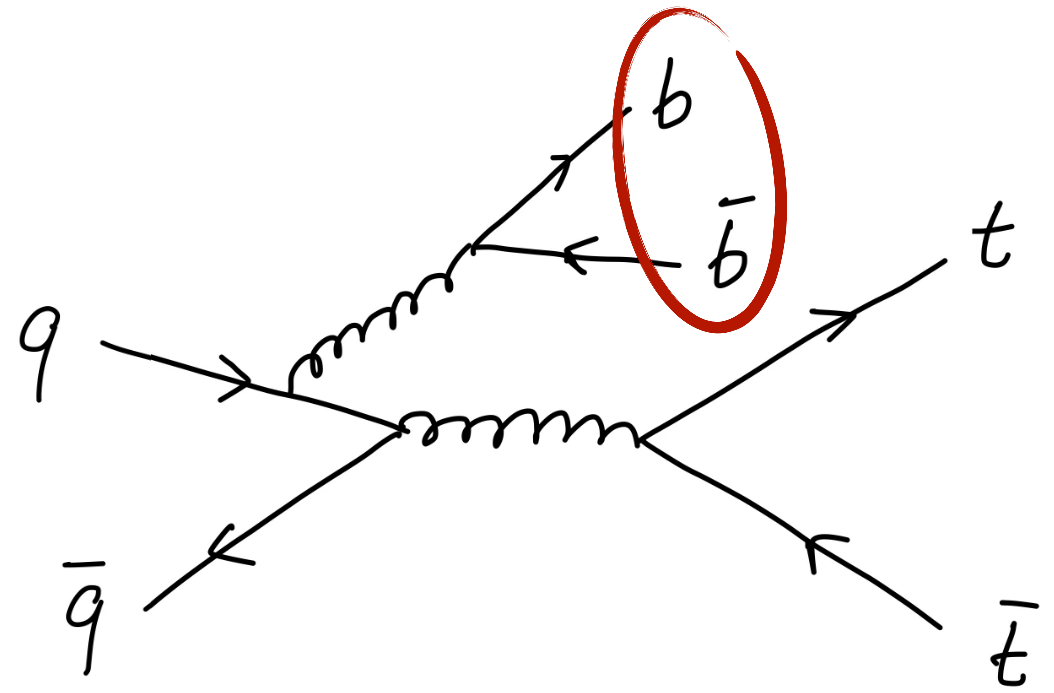


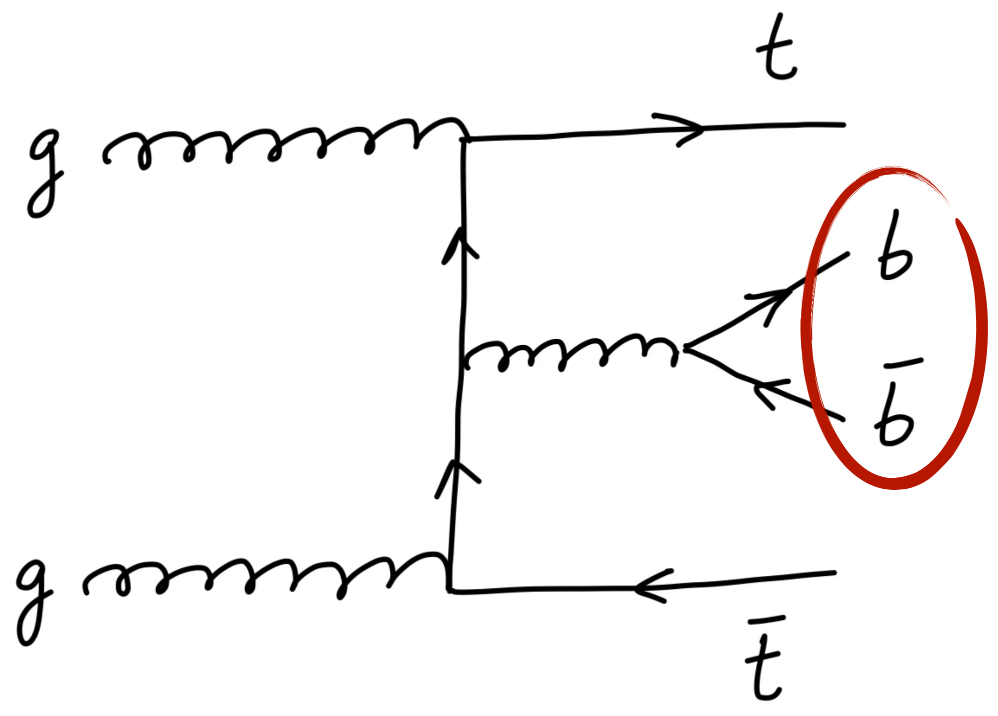
Simulation of the $t\bar{t}b\bar{b}$ process

- **Two primary theoretical frameworks:** four-flavour scheme (4FS) and five-flavour scheme (5FS)

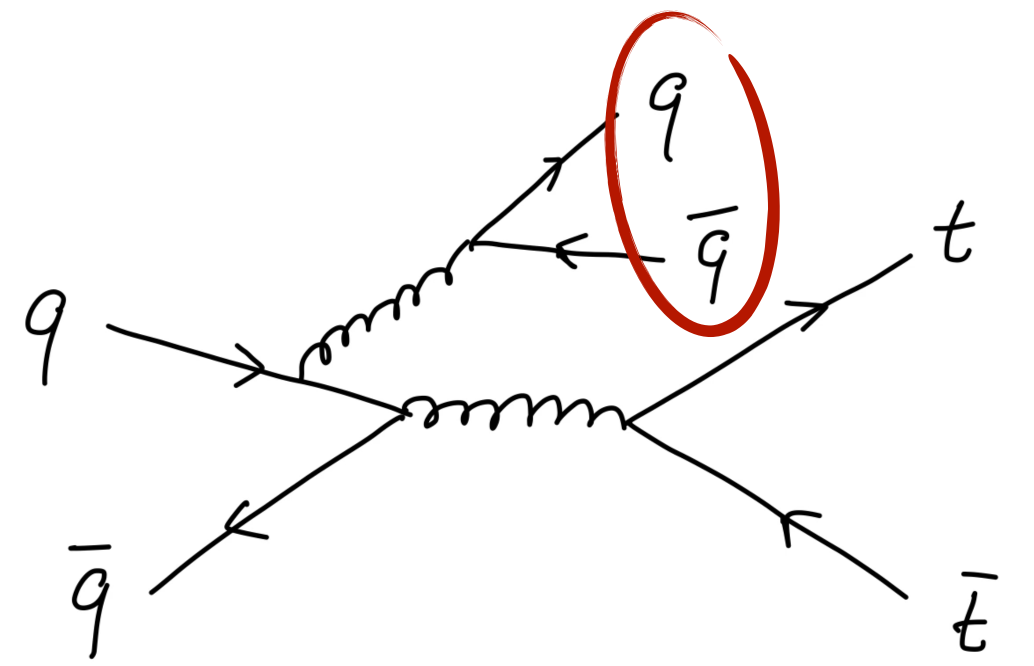
- **Alternative:** “fusion” method (or variable flavor number scheme)
  - Merges aspects of both the 4FS and 5FS calculations
  - Currently, the additional jets are only computed at leading order

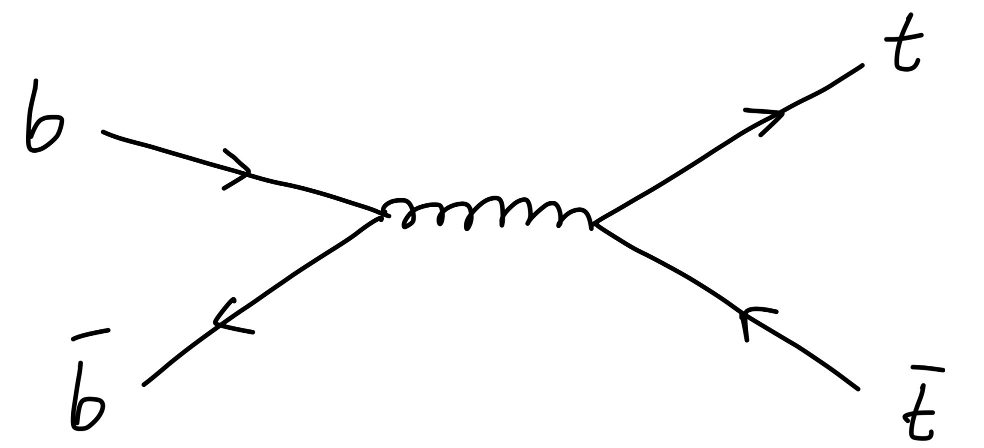
[Höche, Krause, Siegert (2019)](#)
[Ferencz, Höche, Katzy, Siegert (2024)](#)

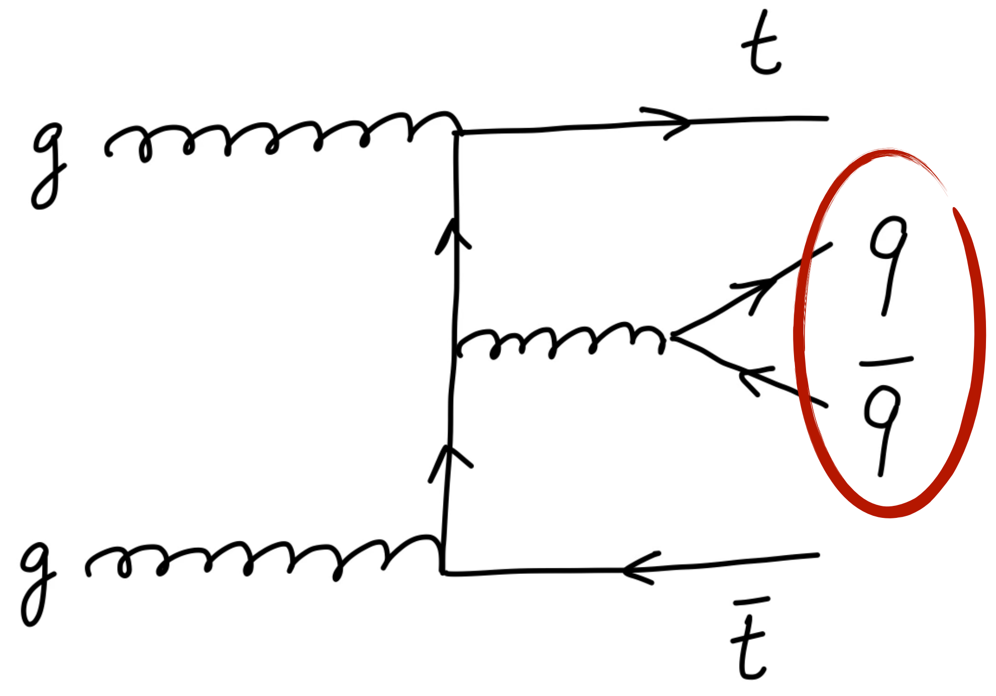




	4FS	5FS
***b*-quarks in the matrix element**	massive	massless
***b*-quarks included in the PDF?**	no	yes
renormalisation scheme	on-shell	$\overline{\text{MS}}$
final state	exclusively $t\bar{t}b\bar{b}$	inclusive $t\bar{t}$ + jets







Simulation of the $t\bar{t}b\bar{b}$ process in the 4FS

- 4FS calculations are usually the most precise at fixed order
  - b-quark mass effects taken into account
  - The processs can be generated down to any energies

Bredenstein, Denner, Dittmaier, Pozzorini (2008)
Bredenstein, Denner, Dittmaier, Pozzorini (2009)
Bevilacqua, Czakon, Papadopoulos, Pittau, Worek (2009)
Buccioni, Kallweit, Pozzorini, Zoller (2019)
Bredenstein, Denner, Dittmaier, Pozzorini (2010)
Denner, Lang, Pellen (2021)
Bevilacqua, Bi, Hartanto, Kraus, Lupattelli, Worek (2021)
Bevilacqua, Bi, Hartanto, Kraus, Lupattelli, Worek (2023)

- Calculation with a certain number of jets at fixed order is reliable only if there are no scale hierarchies
  - $t\bar{t}b\bar{b}$ production is a multi-scale process
  - Large mass difference between the top and bottom quarks → **large logarithms** $\log^n(m_b/\sqrt{s})$
  - Difficult to choose optimal renormalisation and factorisation scales
    - Need a very small μ_R and a small $\mu_F \neq \mu_R$

see the discussion in the LHC Higgs Xsec WG report arXiv:1610.07922

- Challenges arise when matching to a parton shower:
  - Parton shower radiation can produce additional b-quarks
  - Jets generated by the shower can be harder than the matrix-element-level bottom quarks
  - We need only the subleading b-quarks to come from the parton shower, but not the leading ones
    - Not fully understood how the parton shower radiation should be constrained

Cascioli, Maierhöfer, Moretti, Pozzorini, Siegert (2014)
Ježo, Lindert, Moretti, Pozzorini (2018)

Simulation of the $t\bar{t}b\bar{b}$ process in the 5FS

- Generate an inclusive $t\bar{t}$ + jets sample, select b-jets after parton showering

Frixione, Nason, Webber (2003)
Frixione, Nason, Ridolfi (2007)
Hoeche, Krauss, Maierhoefer, Pozzorini, Schonherr, Siegert (2015)
Mazzitelli, Monni, Nason, Re, Wiesemann, Zanderighi (2022)

- Massless b-quarks → **large logarithms do not arise in the matrix element**
- Large scale hierarchies between the top quarks and the jets can be resummed by a multi-jet merging procedure
  - For example, FxFx merging in MadGraph5_aMC@NLO (Frederix, Frixione (2012))
- **Accurate parton-shower approximation for all softer jets**
  - hardest parton shower jets are always softer than the softest matrix element jets, which is not always the case in the 4FS

merging scale

$$p_{\mathrm{T}}(\text{PS jets}) < \mu_Q < p_{\mathrm{T}}(\text{ME jets})$$

except for jets coming from the higher-multiplicity sample

- b-quark mass effects:
  - Important in the collinear/IR region ← incorporated into parton shower splitting fuctions
  - Missing in the matrix element, but they are less relevant for the hard b-quarks

Simulation of the $t\bar{t}b\bar{b}$ process in the 5FS

- But generating $t\bar{t}$ + 0,1,2 jets @ NLO accuracy requires substantional computing resources

Hoeche, Krauss, Schonherr, Siegert (2013) | Frederix, Frixione (2012) | Plätzer (2013)

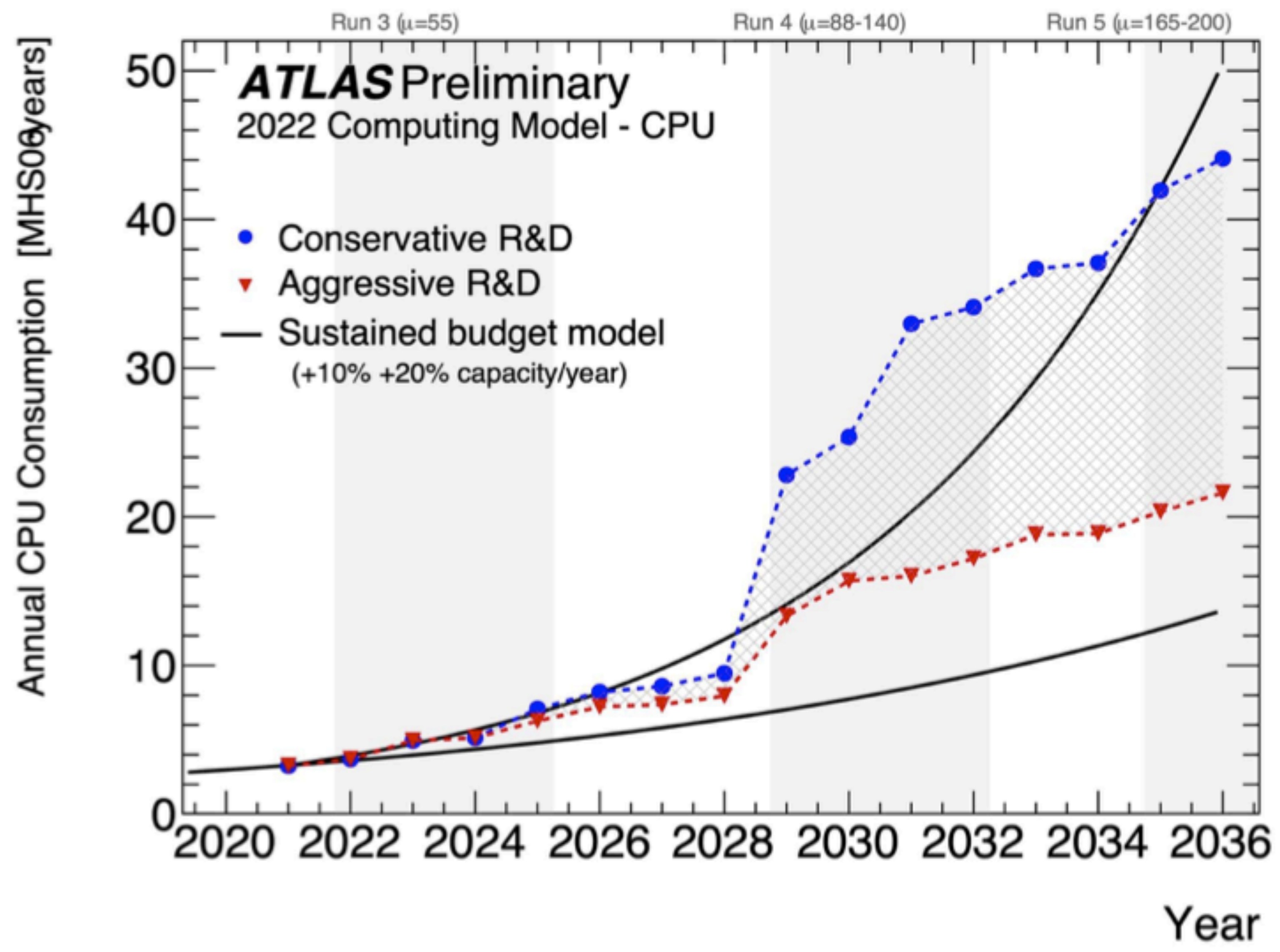
- Selection efficiency of $t\bar{t}b\bar{b}$ is low (percent level)
  - $gg \to t\bar{t}gg$ dominates

number of instructions to calculate a process in MadGraph5_aMC@NLO

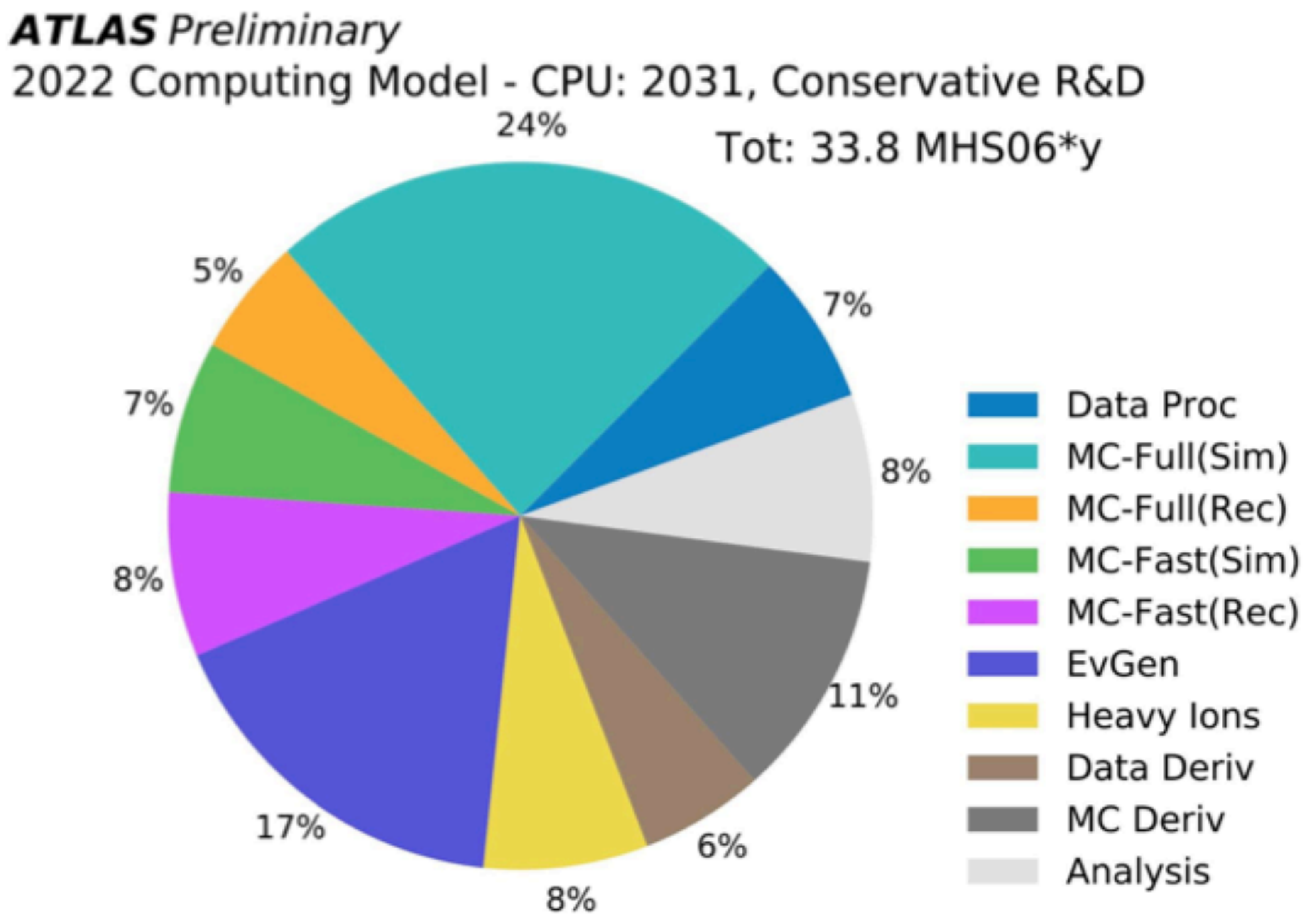
	$gg \to t\bar{t}$	$gg \to t\bar{t}gg$	$gg \to t\bar{t}ggg$
madevent	13G	470G	11T
matrix1	3.1G (23%)	450G (96%)	11T (>99%)
↳ ext	450M (3.4%)	3.3G (<1%)	7.3G (<1%)
↳ int	1.9G (14%)	160G (35%)	2T (19%)
↳ amp	530M (4.0%)	210G (44%)	5.5T (51%)

from O. Mattelaer's talk

➡ **5FS approach is computationally demanding!**
- This will become even more relevant when producing Monte-Carlo for the HL-LHC era



CERN-LHCC-2022-005



b-flavour enhancement in the matrix element

✓ We proposed a novel method to enhance the b-jet selection efficiency in the 5FS approach

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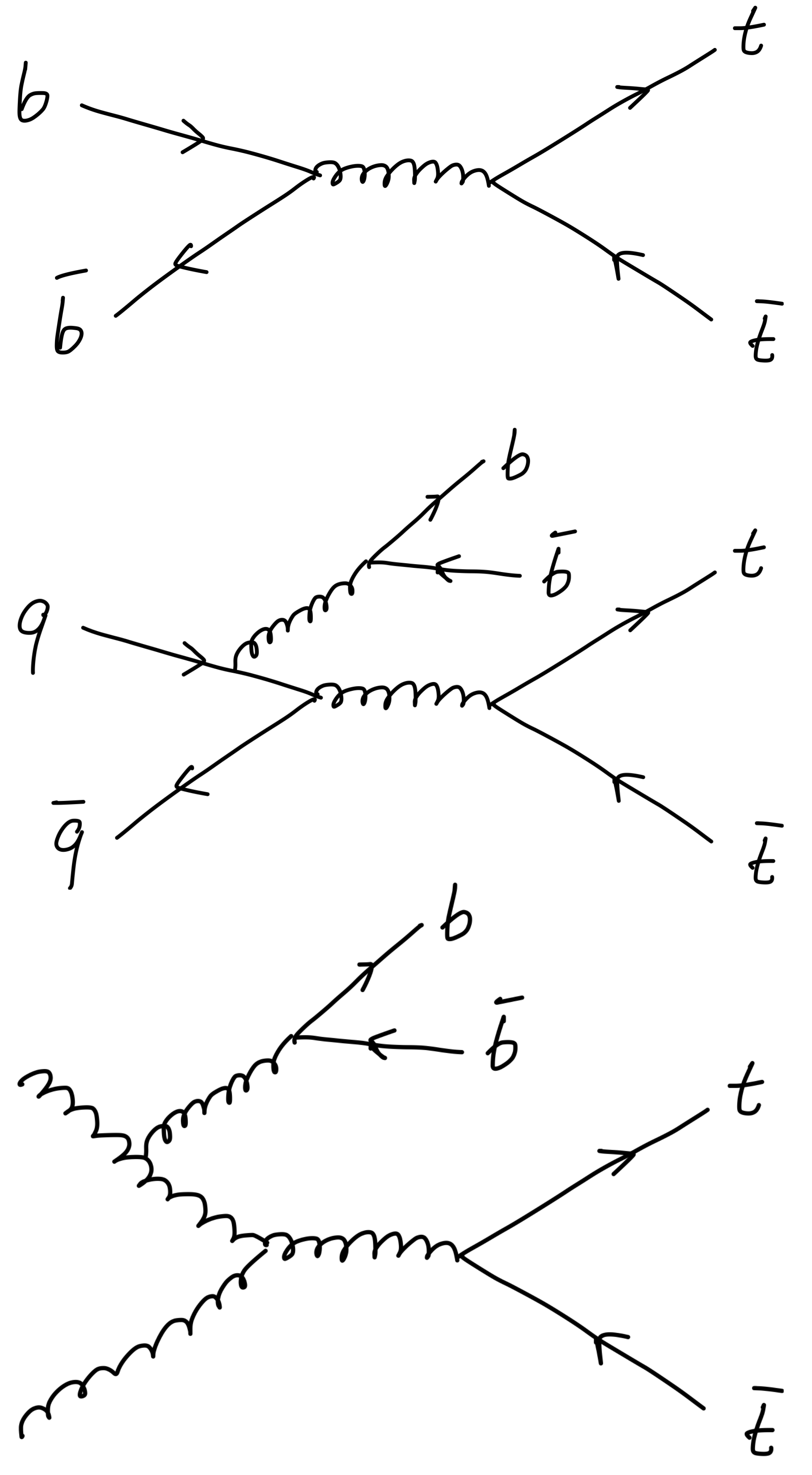
- Augment the generation probability of bottom quark flavour in the short-distance event generation
  - During phase-space integration and unweighting, multiply the weight of each contribution containing external b-quarks by w_{enh}
  - For bottom quarks can be generated in the initial or final state
    - $gg \to t\bar{t}b\bar{b}(g)$
    - $gb \to t\bar{t}bg(\to b\bar{b})$
    - $bb \to t\bar{t}q\bar{q}(g)$

    ...
- To compensate for this and to preserve the cross-section, multiply the weight of events with external b-quarks by $1/w_{\text{enh}}$



examples of the enhanced subprocesses

b-flavour enhancement in the matrix element

✓ We proposed a novel method to enhance the b-jet selection efficiency in the 5FS approach

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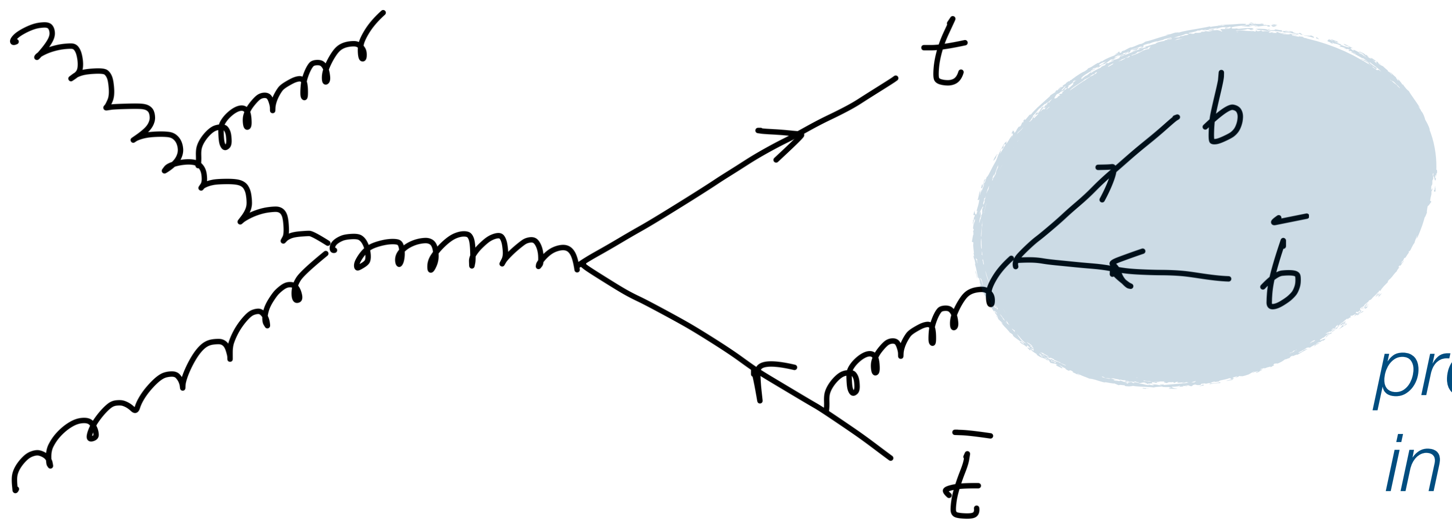
- This procedure is implemented in the MadGraph5_aMC@NLO
  - enhancement factor w_{enh} can be set by a new parameter, `bflav_enhancement`, in the runcard file
  - **The new feature will become part of an upcoming release**

✴ ***NB:*** *hard processes like* $gg \to t\bar{t}gg$ *which can yield a* $t\bar{t}b\bar{b}$ *event after a* $g \to b\bar{b}$ *splitting in the parton shower will not get enhanced* $\Rightarrow$ *the fraction of* $t\bar{t}b\bar{b}$ *events is increased by a factor smaller than* w_{enh}

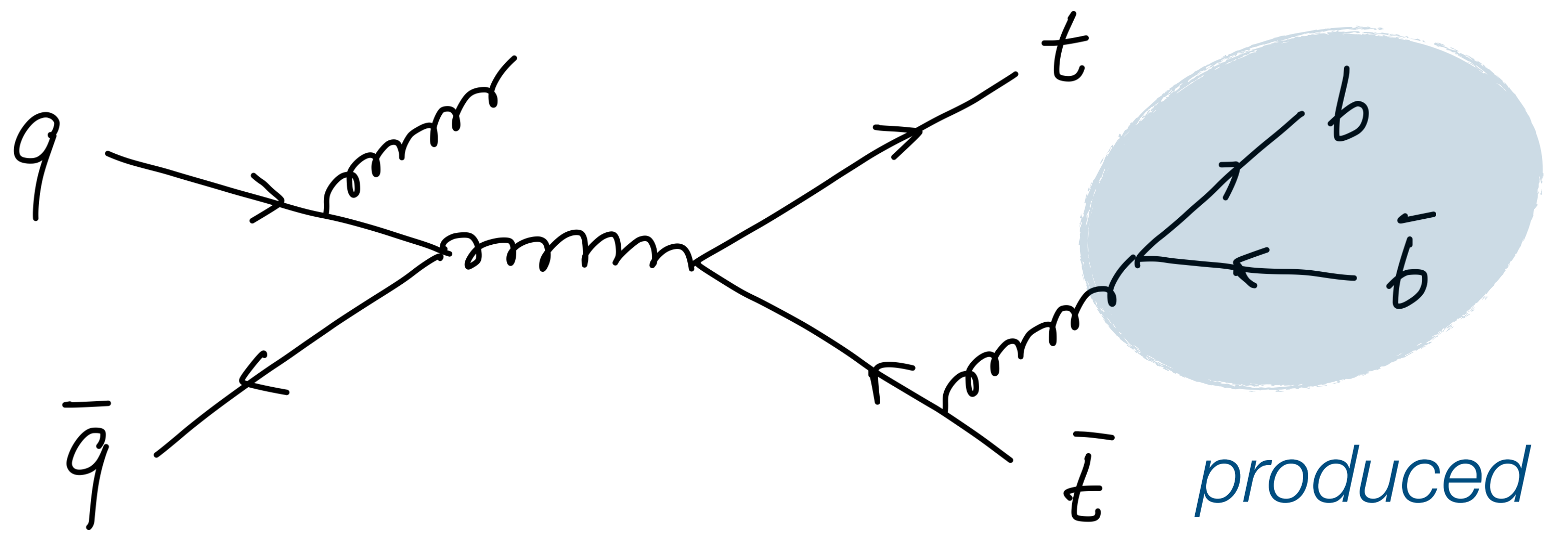
- *also, too high enhancement factors (>100) cause instabilities which result in large statistical fluctuations*



this diagram is not enhanced
— can we enhance it in the PS?

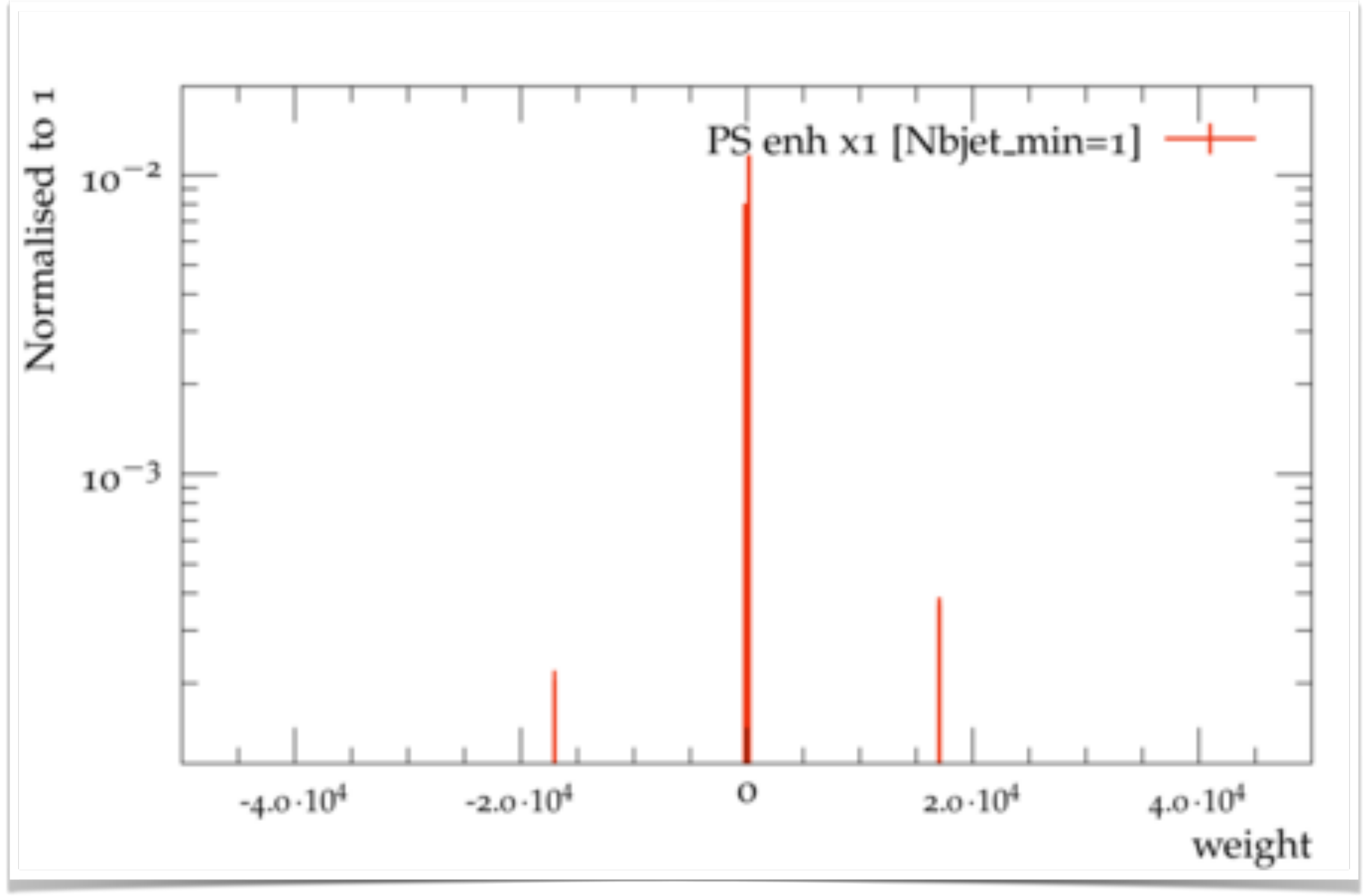
b-flavour enhancement in the parton shower?

- A similar biasing strategy can be potentially applied in the parton shower
- Pythia8 has a built-in mechanism for enhancing splitting probabilities, in particular $g \to b\bar{b}$ ones
  - In versions ≥8.311
- In practice:
  - Even moderate enhancement in the PS causes significant widening of the event weight distribution
  - **Large weights deteriorate the statistics** → cancels the improvement from the b-enhancement completely



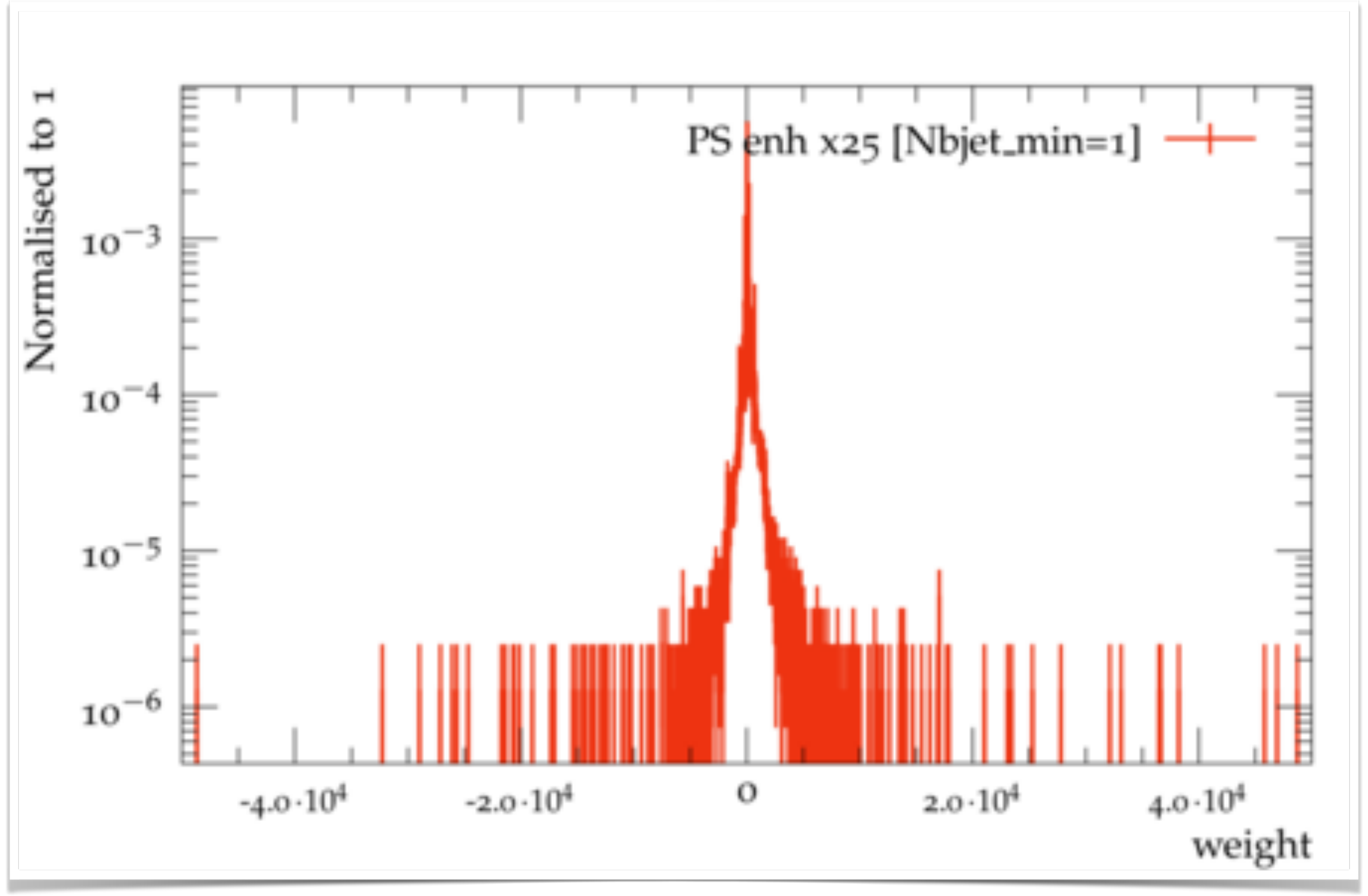
produced in the PS

event weights w/o enhancement in the PS



$g \to b\bar{b}$ enhancement →

event weights with enhancement in the PS



Generation setup for the 5FS sample and comparison to the 4FS

5FS $t\bar{t}$ + jets sample with b-enhancement in the ME

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- **MadGraph5_aMC@NLO $t\bar{t} + 0{,}1{,}2$ jets @NLO sample, FxFx merged**
- **Enhancement factor $w_{\mathrm{enh}} = 100$**
- **Renormalisation/factorisation scales:** central values for are taken from the FxFx merging
  - 7-point variations
- **Merging scale:** 40 GeV
  - variations: 70 and 100 GeV
- **Shower starting scale: $H_{\mathrm{T}}/2$**
  - variation: $H_{\mathrm{T}}/4$

taking an envelope as a total uncertainty

- Generation-level cut of 20 GeV on jet p_{T}
- **Matched to the Pythia8 parton shower**
- **Not including**:
  - hadronisation
  - underlying events
  - top quark decay

to reduce the generation time and to simplify the analysis, and because we focus on the differences in the ME

Truth-level analysis in Rivet:

- anti-k_{T} jets ($R > 0.4$)
  - $p_{\mathrm{T}} > 25$ GeV
  - $|\eta| < 2.5$
- jets containing at least one bottom quark are identified as b-jets
- consider two scenarios:
  - at least 1 b-jet
  - at least 2 b-jets

4FS $t\bar{t}b\bar{b}$ sample

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- **MadGraph5_aMC@NLO+Pythia8** NLO+PS $t\bar{t}b\bar{b}$ sample
- **Renormalisation/factorisation scales**:
  - central values:

$$\mu_R = (E_{T,t} E_{T,\bar{t}} E_{T,b} E_{T,\bar{b}})^{1/4}$$
$$\mu_F = \frac{1}{2}(E_{T,t} + E_{T,\bar{t}} + E_{T,b} + E_{T,\bar{b}})$$

  - 7-point variations

following the recommendations in the LHC Higgs Xsec WG report arXiv:1610.07922

- **Shower starting scale:** $H_T/2$
- Generation-level cut of 20 GeV on jet p_T
- **Matched to the Pythia8 parton shower**
- **Not including**:
  - shower starting scale uncertainty
  - matching scheme uncertainty
  - hadronisation
  - underlying events
  - top quark decay

← *expected to be sizeable, (see the LHCHXSWG report) but is non-trivial to assess exactly*

Truth-level analysis in Rivet:

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  - $p_T > 25$ GeV
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- jets containing at least one bottom quark are identified as b-jets
- consider two scenarios:
  - at least 1 b-jet
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5FS vs 4FS: at least 1 b-jet scenario

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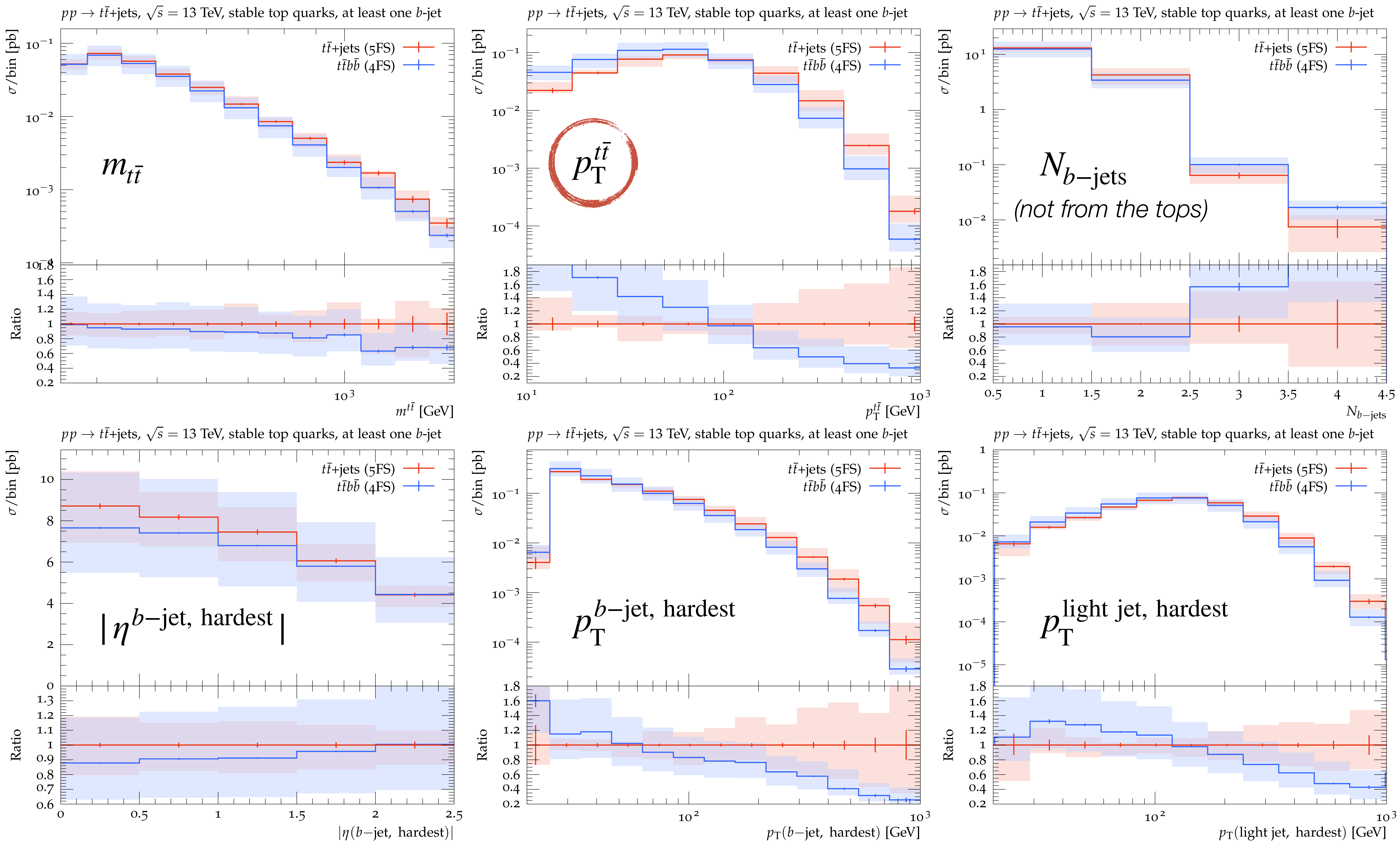
- For most of the variables, 4FS and 5FS predictions are compatible within the uncertainty bands
- 5FS uncertainty is more reliable than the 4FS one, since the 4FS matching uncertainty is expected to be significant but is not included
- The $p_T^{t\bar{t}}$ differs quite a lot, **the 5FS predicts a much harder spectrum than 4FS**
  - ➡ We investigated it further, see next slides



5FS vs 4FS: at least 2 b-jets scenario

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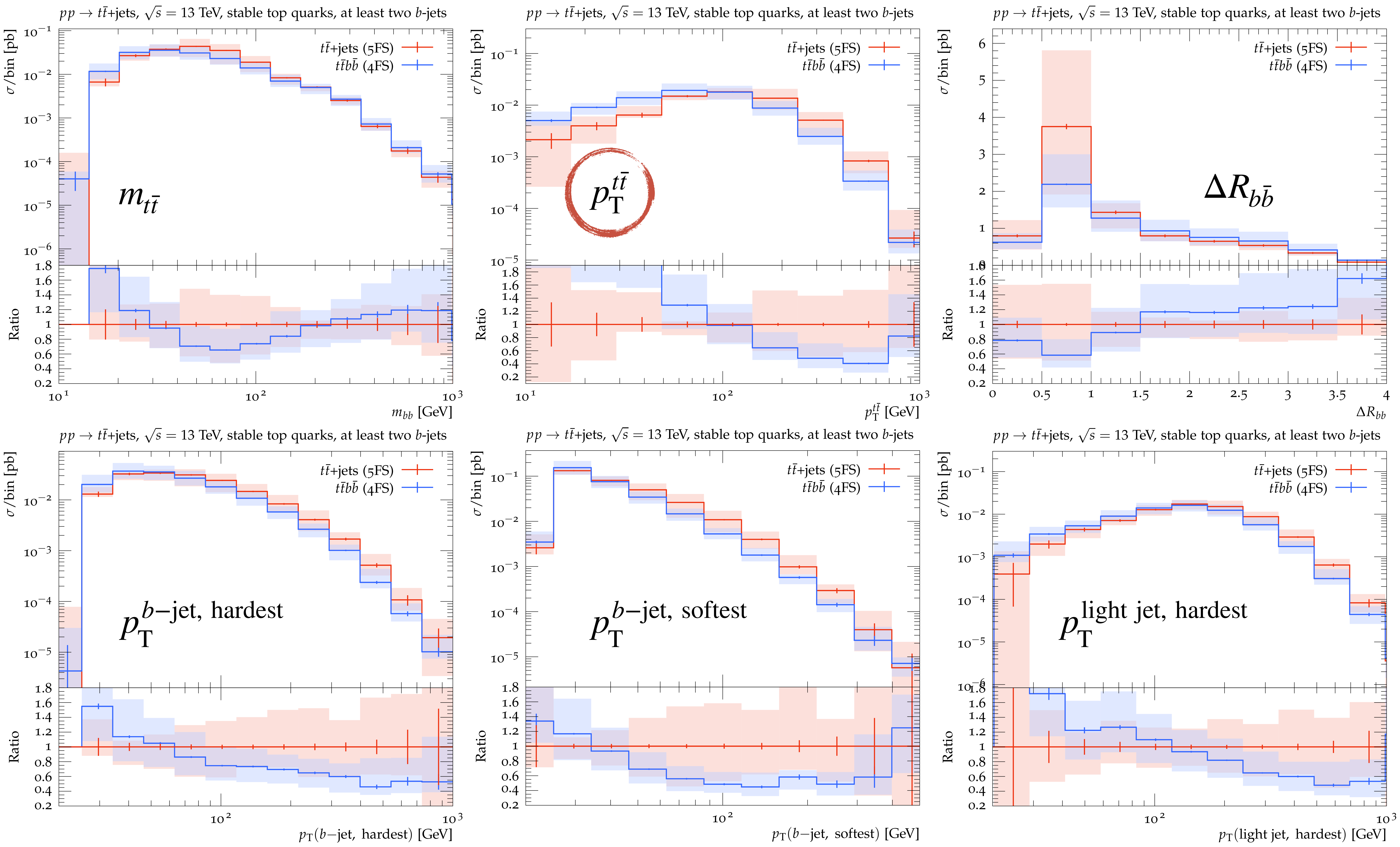
- Similar picture as for the ≥ 1 b-jet selection
- $p_T^{t\bar{t}}$ spectrum differs again
- The rest of the variables are in agreement



5FS vs 4FS: differences in the $p_T^{t\bar{t}}$ distribution

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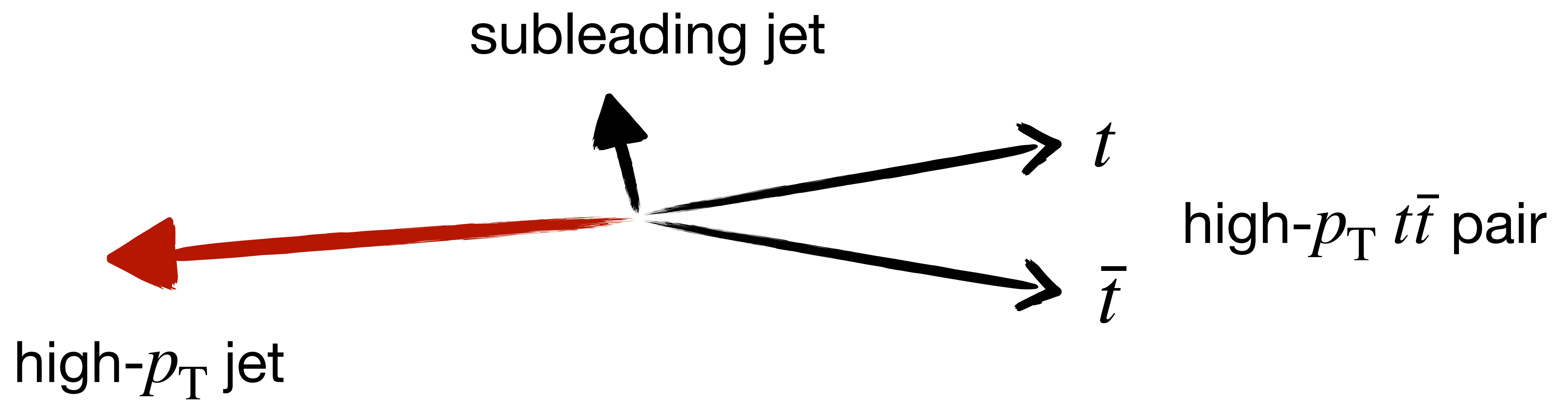
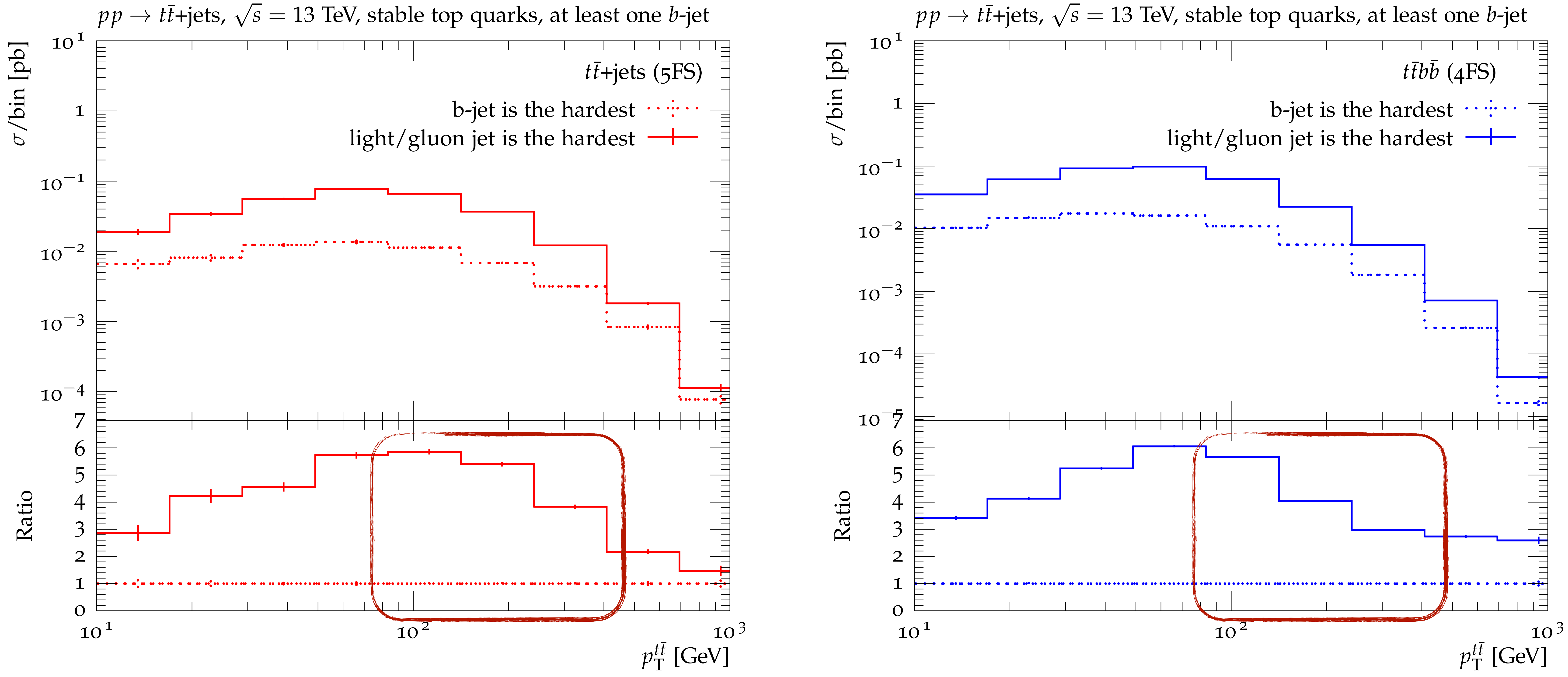
- At large $p_T^{t\bar{t}}$, it is kinematically most-likely that the $t\bar{t}$ pair recoils agains a single hard jet
- If the hardest jet is a light jet:
  - 5FS: described at NLO (most likely it is a gluon jet)
  - 4FS: described at LO or by the PS
    - No $t\bar{t}gg$ events from the ME
    - There is no hard gluon to recoil from



- For high $p_T^{t\bar{t}}$, the fraction of events with the hardest jet being light-flavoured is indeed larger in the 5FS
- But after $p_T^{t\bar{t}} \sim 500$ GeV the situation is opposite — why?
  - Let's look again at the jet p_T distributions…

at least 1 b-jet selection



5FS vs 4FS: differences in the $p_T^{t\bar{t}}$ distribution

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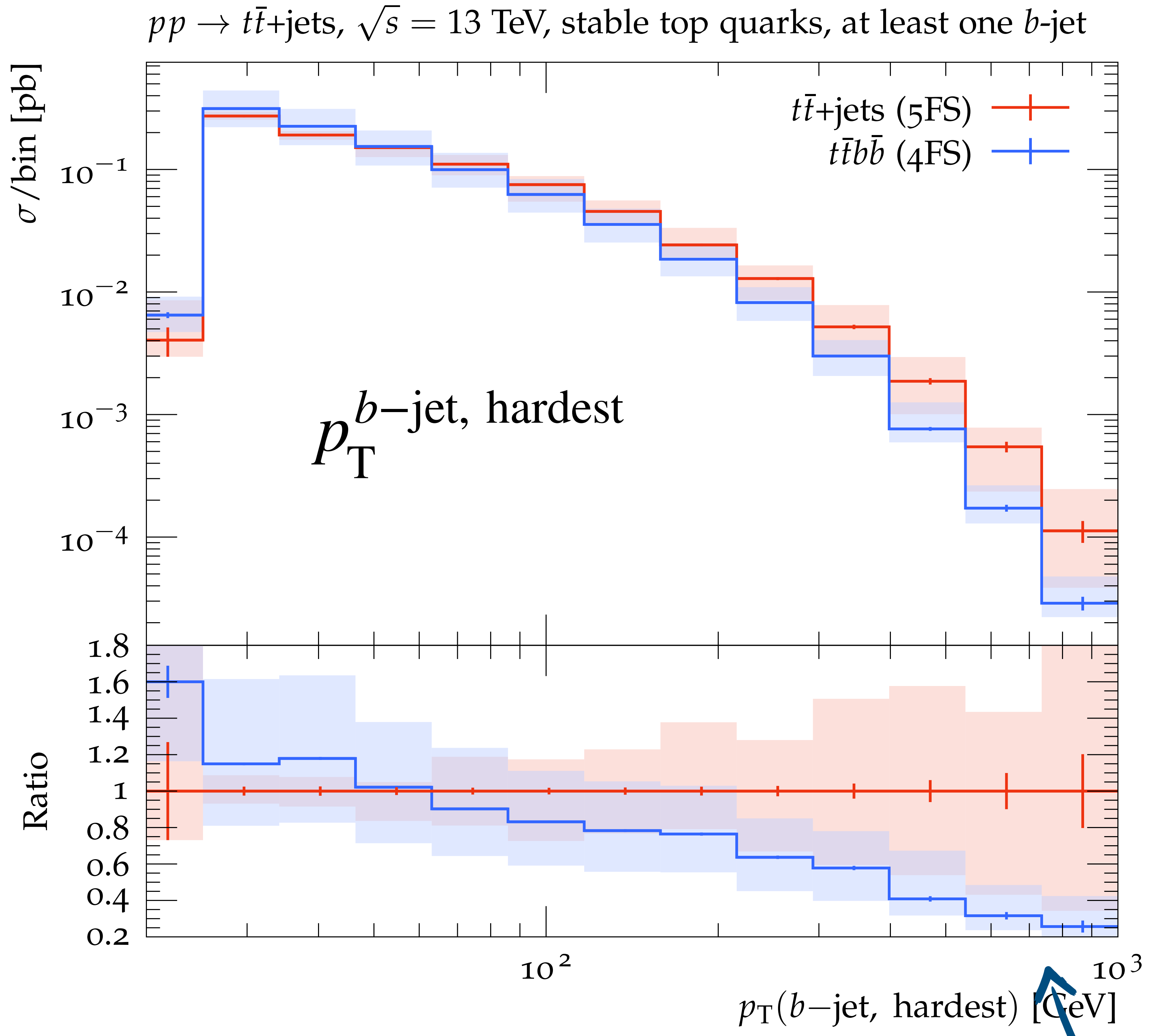

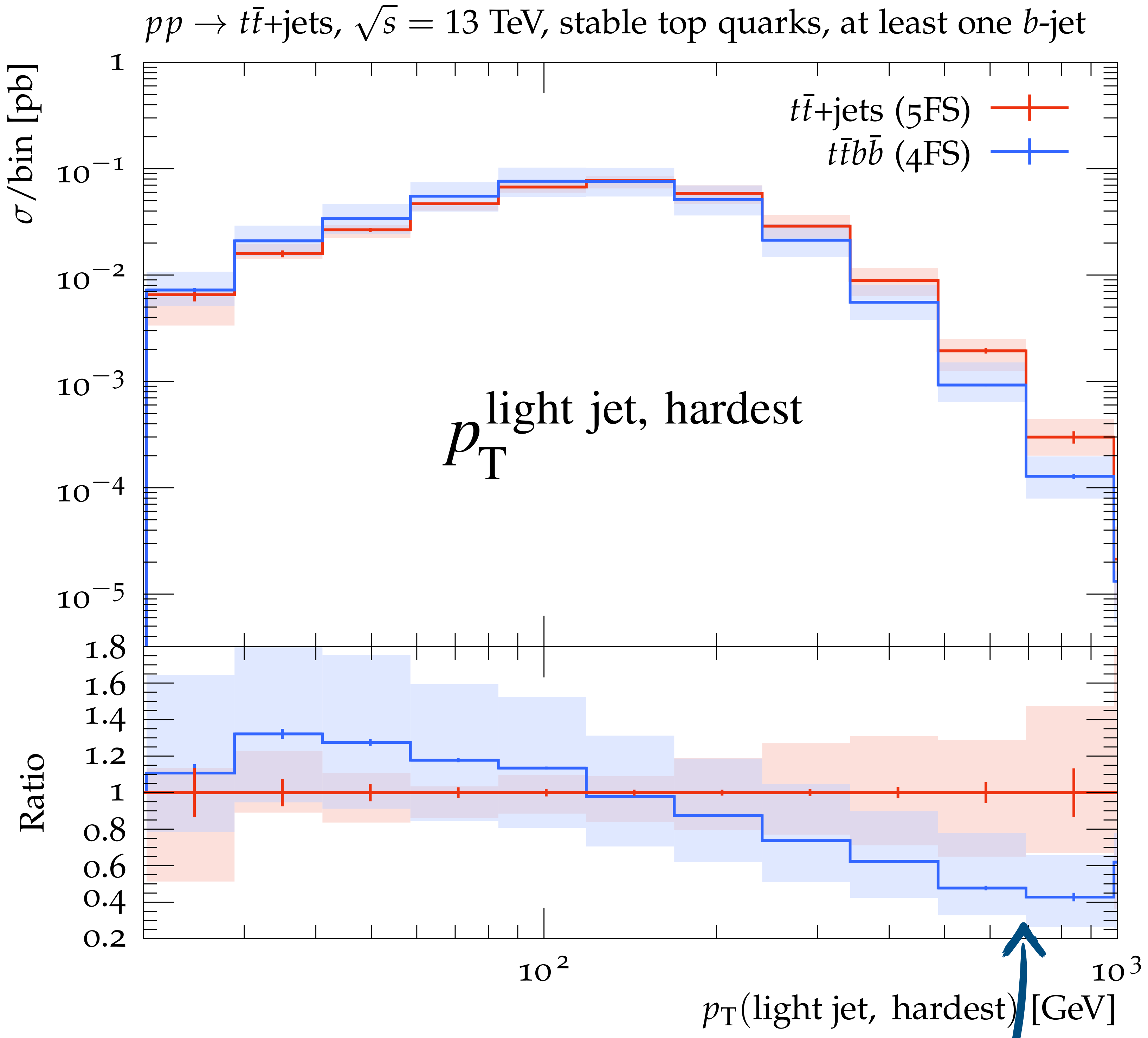

at very high p_T, the ratio of the 5FS over the 4FS predictions is larger for b-jets than for light jets

5FS vs 4FS: differences in the $p_{\mathrm{T}}^{t\bar{t}}$ distribution

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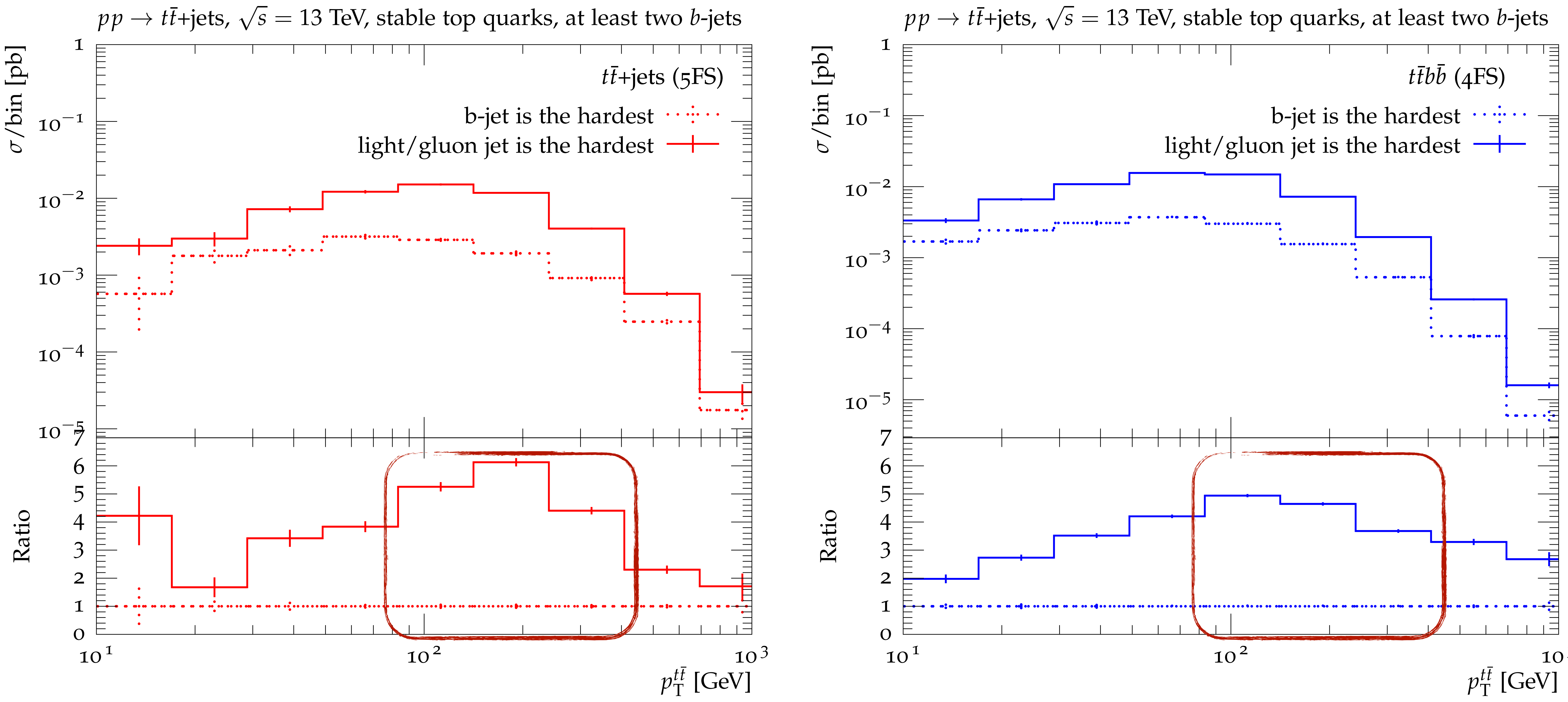
- The difference in the fraction of the hardest light jets in even more pronouced in the ≥ 2 b-jet selection

at least 2 b-jets selection



➡ The reason for the large 5FS–4FS difference in the $p_{\mathrm{T}}^{t\bar{t}}$ spectrum at large momenta is

- The correlation between $p_{\mathrm{T}}^{t\bar{t}}$ and $p_{\mathrm{T}}^{\text{light jet, hardest}}$
- Expected 5FS–4FS difference between the fraction of events with the hardest jet being light-flavoured

To summarise:

- $t\bar{t}b\bar{b}$ production serves as a significant background process across various high-energy physics phenomena
- 5FS calculation of $t\bar{t}b\bar{b}$ at NLO yields the most accurate prediction for this process to date
  - no large logarithms appearing in the matrix element calculation
  - no complications when matching to a parton shower
- We compute the $t\bar{t}$ + jets process with up to 2 jets at NLO using the FxFx merging prescription and match it to the Pythia8 shower
- To improve the efficiency of selecting events with additional b-jets we enhance the probability of producing short-distance events with additional b-quarks using a newly implemented feature in the MadGraph5_aMC@NLO generator
  - This makes producing the $t\bar{t}b\bar{b}$ in the 5FS at NLO more viable, given the computational demands of the 5FS approach

✳ *Similar heavy-flavour enhancement could also be applied to the "fusion" method in Sherpa*
  - *Which might help in increasing the accuracy of the computation for the additional jets*

BACK-UP

Alternative approach: Sherpa fusion

Höche, Krause, Siegert (2019)
Ferencz, Höche, Katzy, Siegert (2024)

- $t\bar{t}b\bar{b}$ merged with $t\bar{t}$+jets in a variable flavour number scheme
- Should have at least the same precision as 5FS, if computed at the same order
- Up to now, the additional jets in the 5FS component are only computed at LO
- Similar 4FS vs 5FS differences as we see in MadGraph+Pythia8