Matrix-Element Merging — The Complexity Bottleneck

For CKKW-L style merging: (incl UMEPS, NL3, UNLOPS, …)

Need to take **all contributing shower histories into account**.

In conventional parton showers,

Each phase-space point receives contributions from many possible branching "histories" (aka "clusterings")

~ sum over (singular) diagrams $\Longrightarrow$ full singularity structure ✅

Number of Histories for n Branchings

Starting from a single $q\bar{q}$ pair	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$
CS Dipole	2	8	48	384	3840	46080	645120

# of histories grows ~ # of Feynman Diagrams, **faster than factorial**

Bottleneck for merging at high multiplicities (+ high code complexity)

Sector Showers (shown without maths)

Skands & Villarejo JHEP 11 (2011) 150 Brooks, Preuss, Skands JHEP 07 (2020) 032

The Default Shower in VINCIA is unique in being a "Sector Shower"

We divide N-gluon Phase Space into N "sectors", with step functions.

Each PS sector corresponds to one specific gluon being the "softest" in the event — the one you would cluster if you were running a jet algorithm (specifically one called ARCLUS)

Inside each sector, **only a single kernel is allowed to contribute** (the most singular one)!

Sector Kernel = the eikonal for the soft gluon and its collinear DGLAP limits for z > 1/2.

The crucial aspect:

Only a single (product of) kernel(s) contributes to each phase-space point

➤ **a single history!**

$\Longrightarrow$ Factorial growth of number of histories reduced to constant!

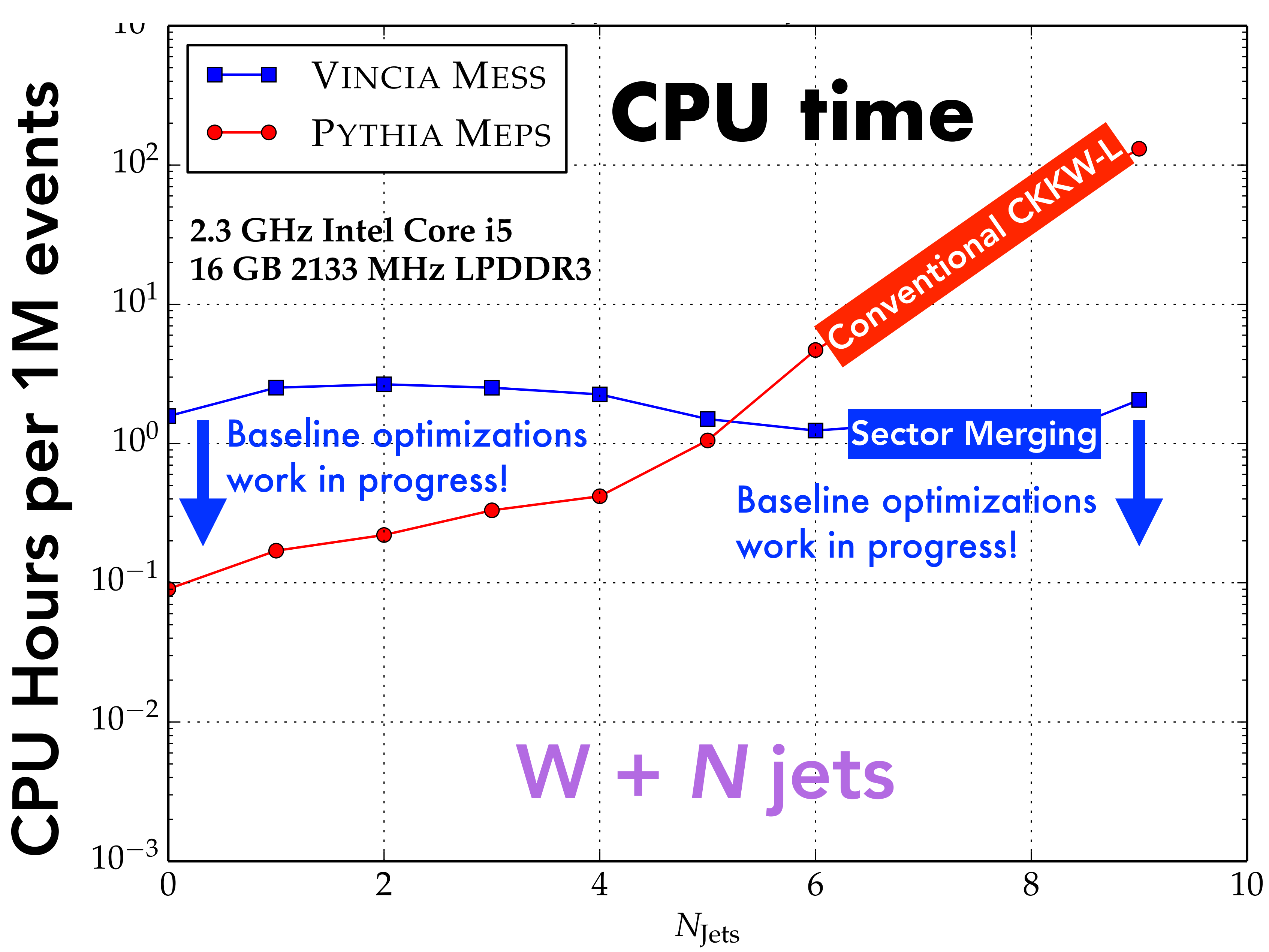
(And the number of sectors only grows linearly with the number of gluons)

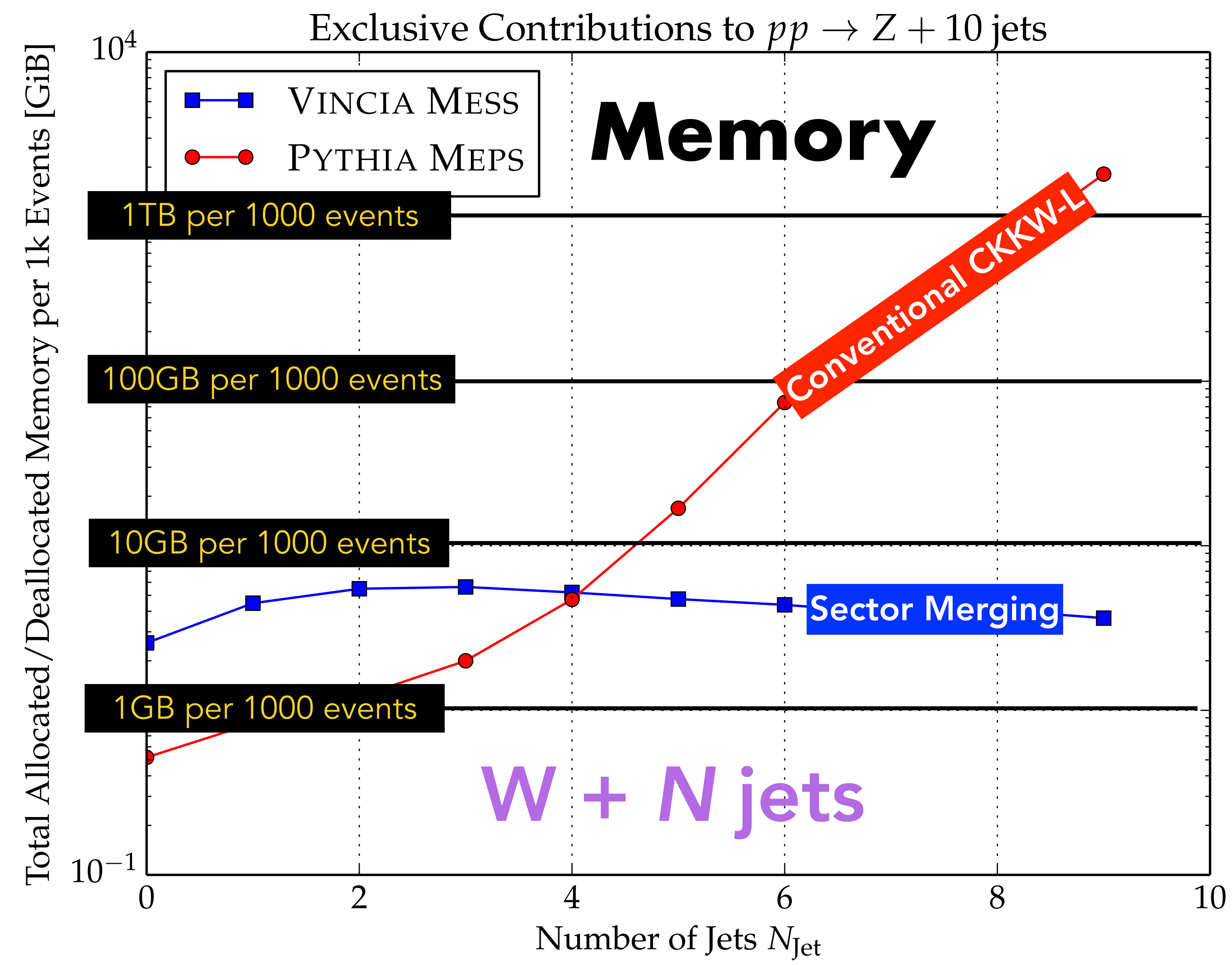
(Once $g \to q\bar{q}$ is included, there is a leftover factorial in number of *same-flavour* quarks; not a big problem)

Sector Merging with VINCIA Sector Shower — Tree Level

Sectorized CKKW-L Merging publicly available from Pythia 8.306

Brooks & Preuss, "Efficient multi-jet merging with the VINCIA sector shower", arXiv:2008.09468





Extensions now pursued:

Sectorized **matching at NNLO** (proof of concepts in arXiv:2108.07133 & arXiv:2310.18671)

Sectorized **iterated tree-level ME corrections** (demonstrated in PS & Villarejo arXiv:1109.3608)

Sectorized **multi-leg merging at NLO**

Preview: VINCIA NNLO+PS for $H \to b\bar{b}$

Coloretti, Gehrmann-de Ridder, Preuss, JHEP 06 (2022) 009

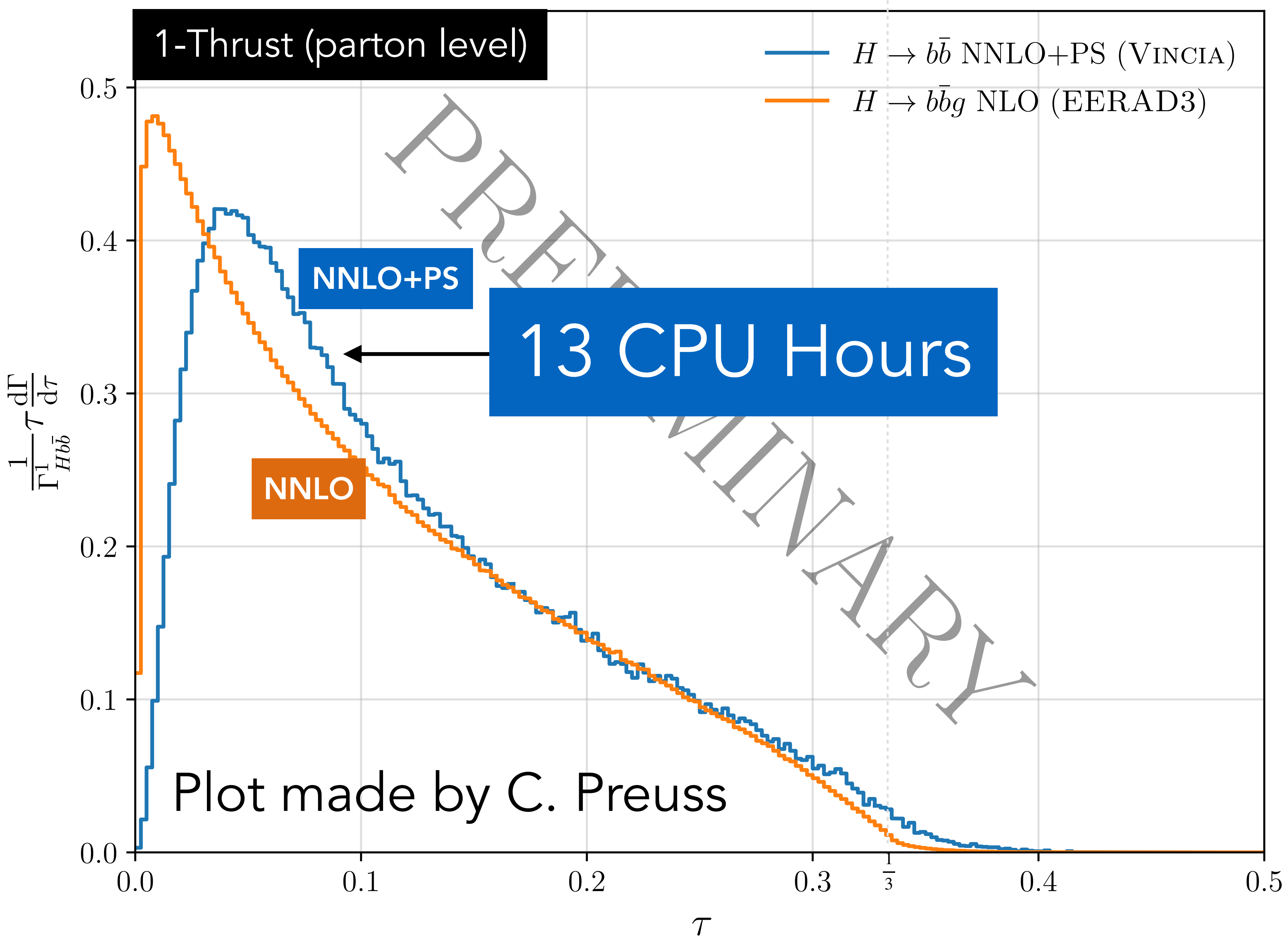
VINCIA NNLO

Fixed-Order Reference = EERAD3 NLO $H \to b\bar{b}g$: already **Highly optimised**

Uses analytical MEs, "folds" phase space to cancel azimuthally antipodal points, and uses antenna subtraction (→ smaller # of NLO subtraction terms than Catani-Seymour or FKS).

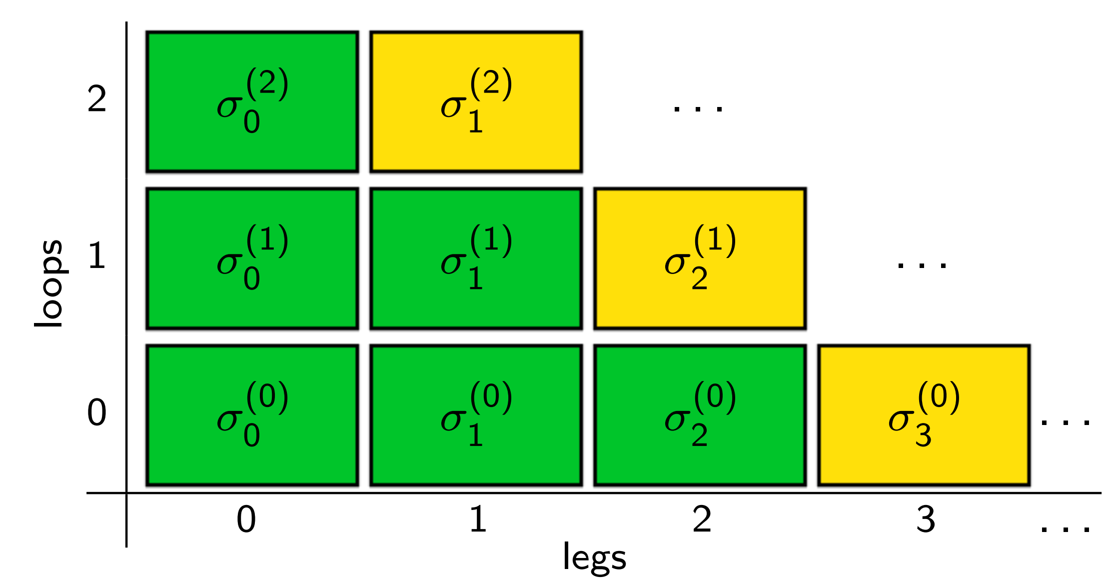
VINCIA NNLO + PS: uses the shower as phase-space generator: **extremely efficient** & everything formulated to be positive definite $\Longrightarrow$ **no negative weights**

➤ **About factor 5 *faster* than EERAD3** (for comparable unweighted stats) + can be hadronised, etc.



Note:

NNLO accuracy in $H \to 2j$ implies **NLO correction in first emission** and **LO correction in second emission.**



So for Thrust,
NNLO $H \to b\bar{b}$
is effectively
NLO for $\tau < 1/3$
LO for $\tau > 1/3$

Expectation: VINCIA NLO MEC approach order-of-magnitude faster than anything less optimised than EERAD3

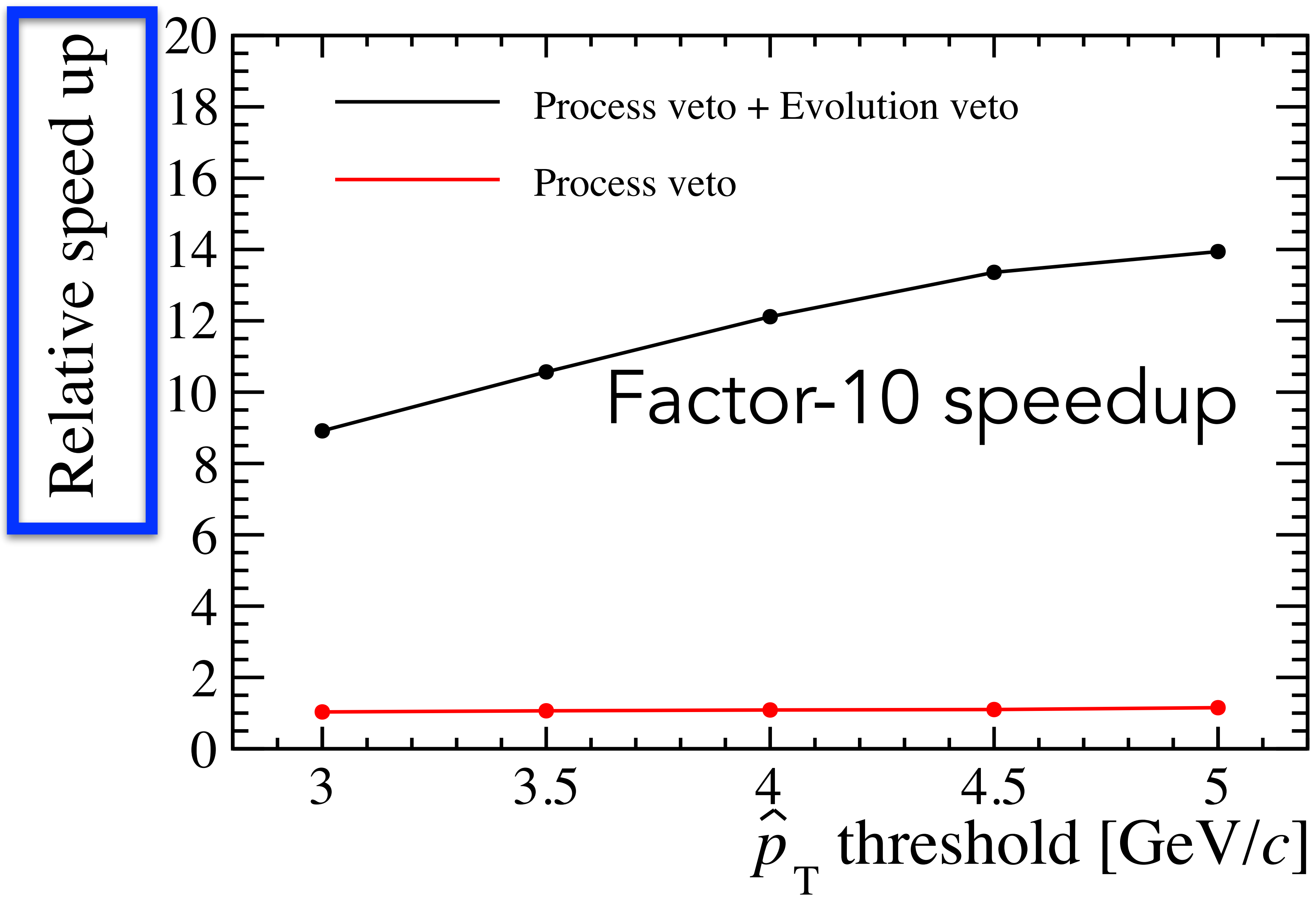
Efficient Heavy-Flavour Physics with PYTHIA

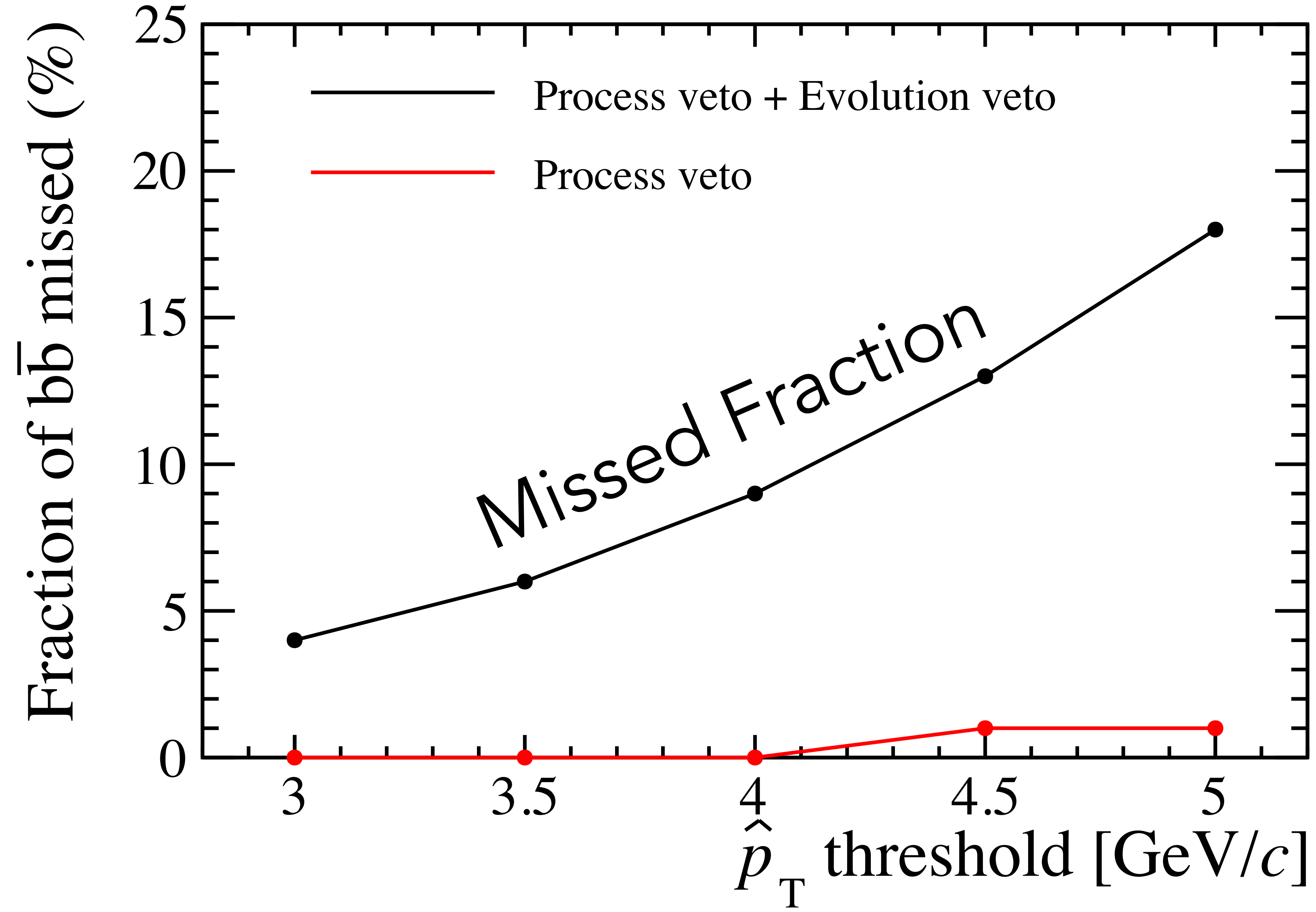
U Egede et al., Eur.Phys.J.C 82 (2022) 9, 773

Production of inclusive samples of specific c and b hadrons can be inefficient, especially if the requested hadrons are rare

New UserHook developed by Monash-Warwick partnership for LHCb

Efficiently veto events that do not contain the requested quarks at the earliest possible stage



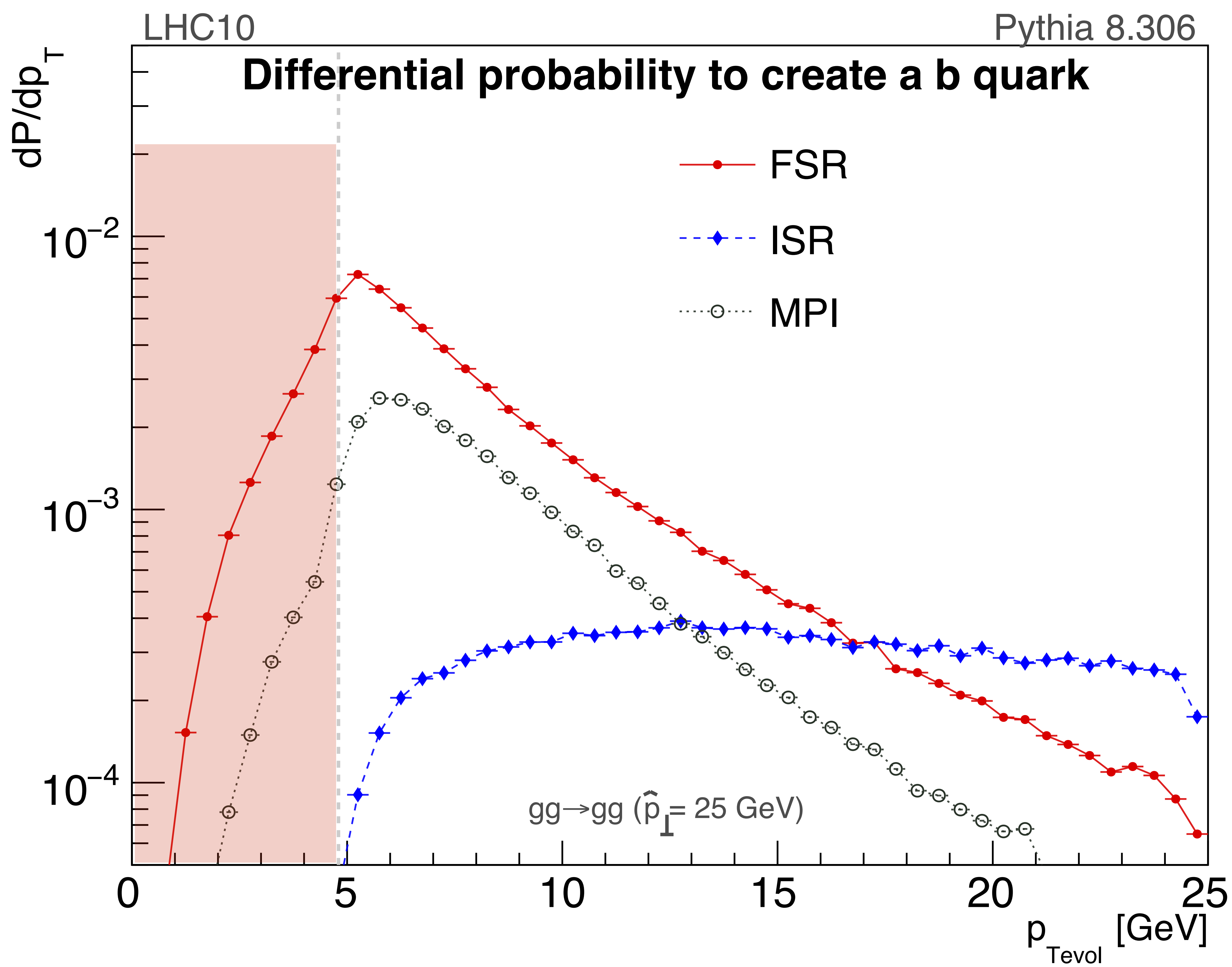


Problem: aggressive speedup misses part of the inclusive *b* cross section

Solution: Revise Evolution Algorithm(s)

U Egede et al., Eur.Phys.J.C 82 (2022) 9, 773

Missed fraction is due to some of PYTHIA's evolution equations allowing b-quarks to be created *below* the b-quark threshold



ISR shows the expected behaviour. Cut at $p_{Tevol} = m_b$ is 100% efficient

FSR and **MPI** both allow b quarks to be created *at scales below* m_b

Work in progres...

Reformulate the **FSR** and **MPI** evolution equations in terms of more physical scales that associate all *b* production with scales above $\mathbf{m_b}$

→ Factor-10 speedup should become 100% efficient

Further ideas: heavy-flavour hadrons on demand? Forced hadronization with weights.

More on Heavy Flavour

QED Corrections in Hadron Decays

SHERPA and HERWIG both have internal YFS-based models

For PYTHIA, QED radiation in hadron decays normally by **PHOTOS**

PHOTOS is beginning to show its age

Experiments report issues with FORTRAN preventing efficient multi-threading

Difficult to update & implement new/advanced models, eg using state-of-the-art matching and merging techniques

VINCIA [Work in progress…]

Has a novel multipole QED shower, competitive with YFS

- Skands & Verheyen, Phys.Lett.B 811 (2020) 135878

Work ongoing via Monash-Warwick Alliance [F. Abudinen, G. Morgante] to test VINCIA-QED as an alternative module for QED showers in hadron decays

- Would also open for combination with new sophisticated treatment of finite-width effects in VINICA: interleaved resonance decays Brooks, Skands & Verheyen, SciPost Phys. 12 (2022) 3, 101

Colour-Reconnection Algorithms — CPU issues

Many measurements have pointed to colour reconnections as a crucial ingredient to model underlying-event and minimum-bias physics

- PYTHIA's default model is too simple; does not reproduce the data
- Alternative QCD CR model [Christiansen & Skands 2015] looks promising
- But nasty combinatorics + implementation issues ➤ significant slowdowns ~ factor 10 relative to default model!

New developments … work in progress …

- M Kreps (Warwick U, via Monash-Warwick Alliance) has analysed the current QCD CR algorithm from general principles
  - Purely code-based modifications look to speed it up by factors 2-3
- Further efficiency gains likely from reconsidering physics implementation
  - Opens door to produce significant event samples with reasonable efficiency
  - Makes new CR model an option to consider for new baseline tunes

Other Thoughts (from P Skands)

Optimisation also crucial to reduce computational footprint / environmental impact

But funders do not (currently) score on this criterion at all

E.g., ERC allow a "Do No Significant Harm" statement — but assessors told **(in boldface)** to ignore it

ARC does not even have such a statement. Not sure about other agencies… ?

Tricky choice if one has to compromise on scientific ambition? Some thoughts on this in *"Computational scientists should consider climate impacts and grant agencies should reward them"*, P Skands, Nature Rev.Phys. 5 (2023) 3, 137-138

All grants I am connected with now include minimisation of footprint as explicit goal

ARC DP22 "Tackling the **computational bottleneck** in precision particle physics" — on **sector-based approaches**

ARC DP23 "Beautiful Strings" — on more **efficient** (and better) models of heavy flavour production, fragmentation, and decays (incl matching), QED showers in hadron decays, collective effects in fragmentation, and Colour Reconnections:

POST DOC AT MONASH NOW OPEN FOR APPLICATIONS

Monash-Warwick Alliance for Particle Physics: including **optimisation and improvements** to **EVTGEN and PYTHIA for HF physics** (incl QED showers and QCD CR)

Royal Society Wolfson Visiting Fellowship "Piercing the **precision barrier** in high-energy particle physics": to develop **efficient techniques for NNLO matching** and beyond + interact with PanScales and with Warwick on **(multithreaded)** multipole **QED showers in hadron decays**

DECRA 23 [L. Scyboz, Monash]**:** "Bridging the accuracy gap: **High-precision parton showers** for colliders" — on **PanScales and VINCIA**.