NNLO+PS predictions for Z boson production in association with b-jets at the LHC

Vasily Sotnikov

University of Zurich

based on

Javier Mazzitelli, VS, Marius Wiesemann [arXiv:2404.08598]

European Research Council
Established by the European Commission

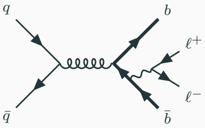
High Precision for Hard Processes (HP2 2024), Turin (Italy)

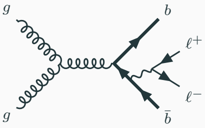
10th September 2024

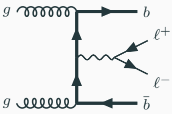
Universität Zürich[UZH]

Introduction

Motivation for $Zb\bar{b}$ production







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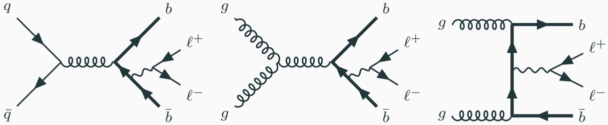
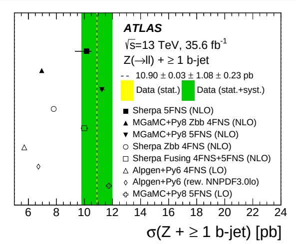


Phenomenological

- Important background to $ZH(bb)$ and BSM searches
- Precision benchmark of pQCD
- Sensitivity to heavy flavor scheme: 4FS vs 5FS



[JHEP 07 (2020) 44]

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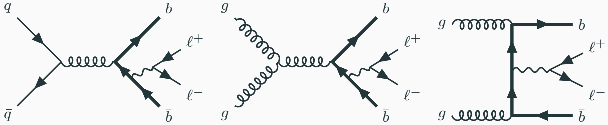

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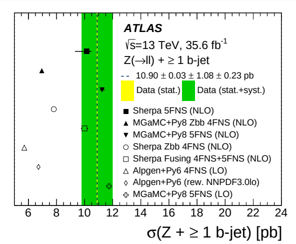

[JHEP 07 (2020) 44]

Technical

- Matching NNLO QCD corrections for a genuine $2 \to 3$ QCD process to parton showers (PS) for the first time
- Extension of a NNLO+PS matching to a new class of processes
- Phenomenological application of one of the most complex two-loop amplitudes known

$Zb\bar{b}$ history

Theory

- NLO 5FS [Campbell, Ellis, Keith, Maltoni, Willenbrock '03]
- NLO 4FS [Febres Cordero, Reina, Wackeroth '08,'09] (see also [Campbell, Ellis, Keith '00])
- NLO+PS in MadGraph5_aMC@NLO [Frederix,Frixione, Hirschi, Maltoni, Pittau, Torrielli '11] (+ multi-jet merging in 5FS)
- NLO+PS in Sherpa [Krauss, Napoletano, Schumann '16] (+ multi-jet merging in 5FS)
- NLO+PS combination 4FS + 5FS [Höche, Krause, Siegert '19] (see also [Forte, Napoletano, Ubiali '18])
- NNLO in 5FS one b-jet [Gauld, Gehrmann-De Ridder, Glover, Huss, Majer '20]

This talk

First NNLO and NNLO+PS computation in 4FS

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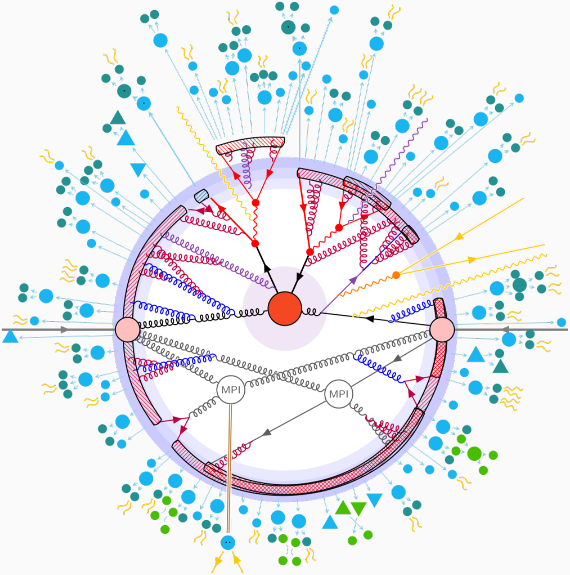
LHC $\sqrt{s} = 13$ TeV measurements

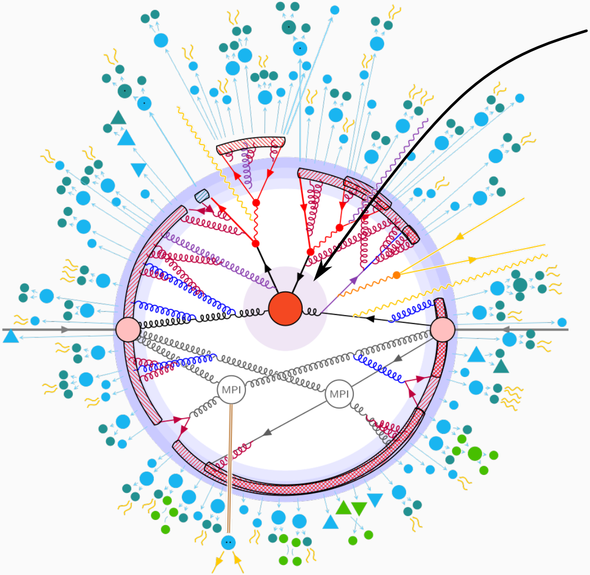
- [ATLAS, arXiv:2003.11960]
- [CMS, arXiv:2112.09659]
- [ATLAS, arXiv:2204.12355] (large R jets)
- [ATLAS, arXiv:2403.15093]

Hadron collisions



[Pythia manual]

Hadron collisions



Hard interaction

✓ N^{x}LO precision

✗ no "events"

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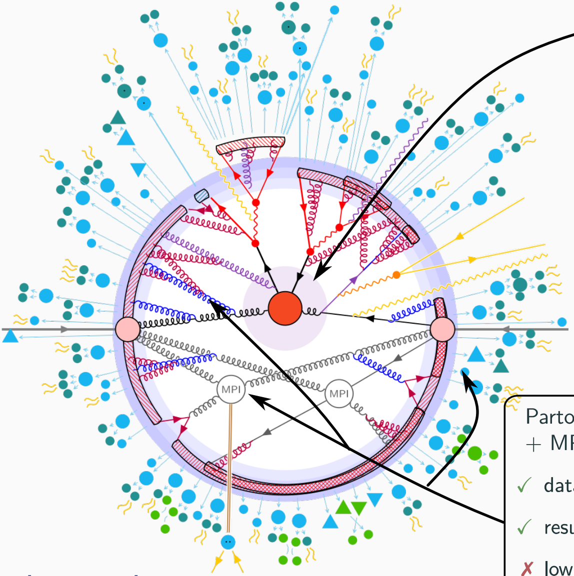

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✓ N^xLO precision

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Parton shower (PS)
+ MPI, hadronization

✓ data-like "events"

✓ resummation of large logarithms

✗ low accuracy

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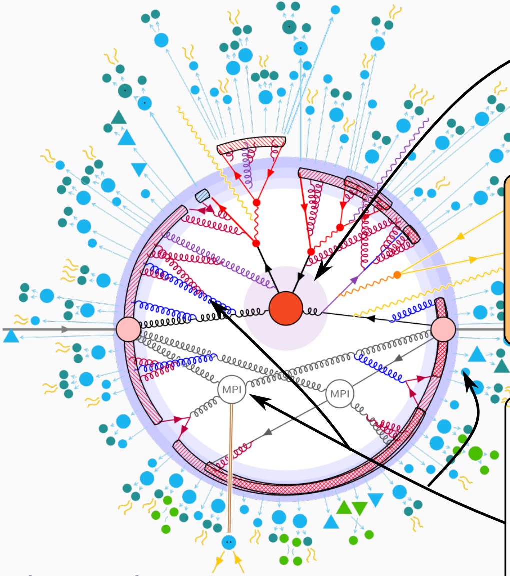

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$N^{x}LO$+PS

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Computational setup

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MiNNLO$_{\mathrm{PS}}$ method

MiNNLO$_{\rm PS}$ for color singlet production

[Monni, Nason, Re, Wiesemann, Zanderighi '19] [Monni, Re, Wiesemann '20]

Step 1: q_T resummation formula

Consider color singlet production $pp \to F + X$

$$\frac{\mathrm{d}\sigma_F^{\text{res}}}{\mathrm{d}\Phi_{\rm F}\mathrm{d}q_T} \sim \frac{\mathrm{d}}{\mathrm{d}q_T}\left\{e^{-S} H \; (C\otimes f)(C\otimes f)\right\}$$

- Differential in Born phase space $\Phi_{\rm F}$ and q_T
- N^{3}LL resummation is NNLO accurate upon integration over q_T

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Step 2: match to Fj @ NLO

$$\mathrm{d}\sigma = \mathrm{d}\sigma_F^{\text{res}} + \left[\mathrm{d}\sigma_{Fj}\right]_{\text{f.o.}} - \left[\mathrm{d}\sigma_F^{\text{res}}\right]_{\text{f.o.}}$$

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Pull out Sudakov exponent, expand to α_s^3:

$$\mathrm{d}\sigma^{\mathrm{MiNNLO}} \sim e^{-S}\ \left(\mathrm{d}\sigma_{Fj}^{(1)}(1 + S^{(1)}) + \mathrm{d}\sigma_{Fj}^{(2)}\ +\ D^{(3)}\right)$$

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Note: e^{-S} exponentially suppresses $q_T \to 0 \implies$ NNLO subtraction

MiNNLO$_{\rm PS}$ for color singlet production

[Monni, Nason, Re, Wiesemann, Zanderighi '19] [Monni, Re, Wiesemann '20]

Step 3: upgrade POWHEG Fj @ NLO generator

$$\mathrm{d}\sigma_{Fj}^{\mathsf{pwg}} = \mathrm{d}\Phi_{\mathrm{Fj}} \;\; \tilde{B}^{Fj} \;\; \times \;\; \left\{ \Delta_{\mathsf{pwg}}(p_T^{\mathsf{min}}) + \mathrm{d}\Phi_{\mathrm{rad}}\, \Delta_{\mathsf{pwg}}(p_{T,\mathsf{rad}}) \frac{R_{Fj}}{B_{Fj}} \right\}$$

$$\tilde{B}_{Fj} \sim \frac{\mathrm{d}\sigma_{Fj}^{\mathsf{NLO}}}{\mathrm{d}\Phi_{\mathrm{Fj}}}$$

- Generates events in Φ_{Fj} distributed according to $\tilde{B}^{Fj}$
- Replace $\tilde{B}^{Fj} \longrightarrow \frac{\mathrm{d}\sigma^{\mathrm{MiNNLO}}}{\mathrm{d}\Phi_{\mathrm{Fj}}}$, such that $\int \mathrm{d}q_T \, \frac{\mathrm{d}\sigma_{Fj}}{\mathrm{d}\Phi_{\mathrm{Fj}}}$ is NNLO accurate

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MiNNLO$_{\mathrm{PS}}$ accuracy

- NNLO for inclusive observables (differential in Φ_{F})
- Resummation from parton shower (PS) preserved (e.g. LL in p_T)
- No unphysical scales

Extension to heavy quark pair (+singlet) production

$pp \to Q\bar{Q} + F$

Resummation structure more complex

[Zhu, Li, Li, Shao, Yang '12] [Catani, Grazzini, Torre '14]

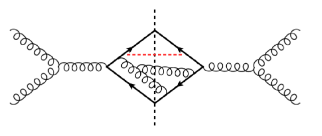
$$d\sigma_F^{\text{res}} \sim \frac{d}{dq_T}\left\{e^{-S} H \; (C \otimes f)(C \otimes f)\right\} \longrightarrow$$

$$d\sigma_{Q\bar{Q}}^{\text{res}} \sim \frac{d}{dq_T}\left\{e^{-S}\left[\text{Tr}[\mathbf{H}\boldsymbol{\Delta}] \; (C \otimes f)(C \otimes f)\right]_{\phi}\right\}$$

- Additional radiative factor $\boldsymbol{\Delta}$ of soft origin [Catani, Devoto, Grazzini, Mazzitelli '23]
- Cast into a sum of color-singlet-like contributions to connect to $\text{MiNNLO}_{\text{PS}}$ formalism [Mazzitelli, Monni, Nason, Re, Wiesemann, Zanderighi '20]
- Explicit integration of (subtracted) soft current required (up to 4-fold numerical integration)

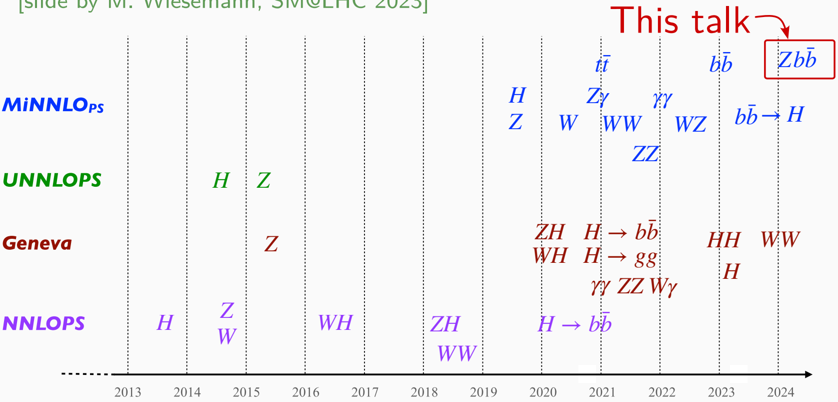
SHARK

[Devoto, Mazzitelli, in preparation]



NNLO+PS timeline

[slide by M. Wiesemann, SM@LHC 2023]



Computational setup

Two-loop corrections

Two-loop hard function

$$e^{-S}\Big[\mathrm{Tr}[\mathbf{H}\boldsymbol{\Delta}]\;(C\otimes f)(C\otimes f)\Big]_\phi \qquad\longrightarrow\qquad H=\frac{\langle\mathcal{R}|\bar{\mathbf{h}}^\dagger\bar{\mathbf{h}}|\mathcal{R}\rangle}{\big|\mathcal{M}^{(0)}\big|^2},\quad |\mathcal{R}\rangle=\mathbf{Z}^{-1}\,|\mathcal{M}\rangle\,,$$

$$\bar{\mathbf{h}}=1+\mathcal{O}(\alpha_s)$$

- Operator $\mathbf{Z}^{-1}=1+\mathcal{O}(\alpha_s)$ absorbs IR divergences [Becher, Neubert '09]
- Two-loop corrections contribute to hard-virtual function H through $2\,\mathrm{Re}\,\big\langle\mathcal{R}^{(0)}\big|\mathcal{R}^{(2)}\big\rangle$
- Need five-point two-loop amplitudes for $q\bar{q}\to Zb\bar{b}$, $gg\to Zb\bar{b}$ with massive b, currently out of reach [see Bayu's talk]

Small m_b expansion

Scale hierarchy $m_b \ll \mu_h \implies$ factorization [Mitov, Moch '06]:

$$|\mathcal{M}\rangle = \mathcal{F}\,|\mathcal{M}_0\rangle \; + \; \mathcal{O}\left(\frac{m_b}{\mu_h}\right), \qquad \mathcal{F}^{(l)} = \sum_{i=0}^{2l} f_i \log\left(\frac{m_b}{\mu_R}\right)^i$$

$$|\mathcal{M}\rangle^{(2)} = \mathcal{F}^{(2)}\left|\mathcal{M}_0^{(0)}\right\rangle + \mathcal{F}^{(1)}\left|\mathcal{M}_0^{(1)}\right\rangle + \left|\mathcal{M}_0^{(2)}\right\rangle$$

Intuition: $1/\epsilon$ poles in 5FS scheme ($|\mathcal{M}_0\rangle$) related to $\log\frac{m_b}{\mu_R}$ power in 4FS ($|\mathcal{M}\rangle$) via "massification".

Application to NNLO $Wb\bar{b}$ production [Buonocore, Devoto, Kallweit, Mazzitelli, Rottoli, Savoini '22]

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Recently extended to include contributions from closed b loops [Wang, Xia, Yang, Ye '23]:

$$\mathcal{F}\,|\mathcal{M}_0\rangle \;\to\; \mathcal{F}'\;\mathbf{S}\,|\mathcal{M}_0\rangle\,,$$

$\mathbf{S} = 1 + \mathbf{S}^{(2)}$ soft function (operator in color space) with additional $\log\frac{m_b}{\mu_R}$ contributions.
[see Guoxing's talk]

Finite formulation of massification

$$|\mathcal{M}\rangle = \mathcal{F}\ \mathbf{S}\ |\mathcal{M}_0\rangle$$

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- Factorization formulated for divergent quantities
- Higher orders in ϵ required in $|\mathcal{M}_0(\epsilon)\rangle$, (e.g. 1-loop to ϵ^2 for NNLO)
- Modern analytic methods compute finite remainders $|\mathcal{R}\rangle = \mathbf{Z}^{-1}\,|\mathcal{M}\rangle$ directly

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Finite formulation

Multiply by $\mathbf{Z}^{-1}_{m_b \ll \mu_h}$ and insert $1 = \mathbf{Z}_0\mathbf{Z}^{-1}$:

$$|\mathcal{R}_{m_b \ll \mu_h}\rangle = \mathbf{Z}^{-1}_{m_b \ll \mu_h}\,\mathcal{F}\,\mathbf{S}\,\mathbf{Z}_0\ |\mathcal{R}_0\rangle\ \ =\ \ \bar{\mathcal{F}}\,\bar{\mathbf{S}}\,|\mathcal{R}_0\rangle$$

$\bar{\mathcal{F}}$, $\bar{\mathbf{S}}$ finite, $\bar{\mathcal{F}}$ diagonal in color space

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Evaluate 2-loop contribution as

$$\mathrm{Re}\left\langle \mathcal{R}_0^{(0)} \middle| \mathcal{R}^{(2)}_{m_b \ll \mu_h} \right\rangle = \bar{\mathcal{F}}^{(2)} \left| \mathcal{R}_0^{(0)} \right|^2 + \bar{\mathcal{F}}^{(1)}\,\mathrm{Re}\left\langle \mathcal{R}_0^{(0)} \middle| \mathcal{R}_0^{(1)} \right\rangle + \mathrm{Re}\,\left\langle \mathcal{R}_0^{(0)} \middle| \bar{\mathbf{S}}^{(2)} \middle| \mathcal{R}_0^{(0)} \right\rangle + \mathrm{Re}\left\langle \mathcal{R}_0^{(0)} \middle| \mathcal{R}_0^{(2)} \right\rangle$$

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$\log(m_b)$ terms

Further approximations

$$\mathrm{Re}\left\langle \mathcal{R}_0^{(0)} \middle| \mathcal{R}_{m_b \ll \mu_h}^{(2)} \right\rangle =$$
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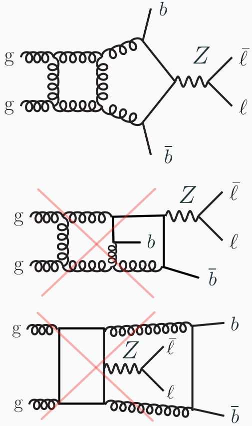
Massless two-loop $pp \to Zb\bar{b}$ process simpler, still on the cutting edge. We evaluate $\mathrm{Re}\left\langle \mathcal{R}_0^{(0)} \middle| \mathcal{R}_0^{(2)} \right\rangle$ based on analytic results [Abreu, Febres Cordero, Ita, Klinkert, Page, VS '21] [Chicherin, VS, Zoia '21]

- Leading color approximation ($1/N_c^2$ supressed)
- Contributions with Z coupling to closed quark loops discarded (estimated negligible at NLO).



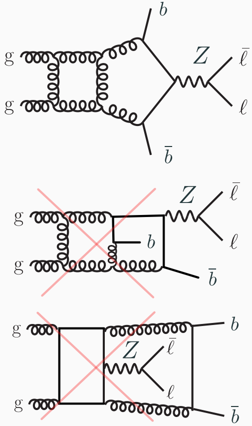
Further approximations

$$\mathrm{Re}\left\langle \mathcal{R}_0^{(0)} \middle| \mathcal{R}^{(2)}_{m_b \ll \mu_h} \right\rangle =$$

$$\bar{\mathcal{F}}^{(2)} \left| \mathcal{R}_0^{(0)} \right|^2 + \bar{\mathcal{F}}^{(1)}\, \mathrm{Re}\left\langle \mathcal{R}_0^{(0)} \middle| \mathcal{R}_0^{(1)} \right\rangle + \mathrm{Re}\left\langle \mathcal{R}_0^{(0)} \middle| \bar{\mathbf{S}}^{(2)} \middle| \mathcal{R}_0^{(0)} \right\rangle + \mathrm{Re}\left\langle \mathcal{R}_0^{(0)} \middle| \mathcal{R}_0^{(2)} \right\rangle$$

Massless two-loop $pp \to Zb\bar{b}$ process simpler, still on the cutting edge. We evaluate $\mathrm{Re}\left\langle \mathcal{R}_0^{(0)} \middle| \mathcal{R}_0^{(2)} \right\rangle$ based on analytic results [Abreu, Febres Cordero, Ita, Klinkert, Page, VS '21] [Chicherin, VS, Zoia '21]

- Leading color approximation ($1/N_c^2$ supressed)
- Contributions with Z coupling to closed quark loops discarded (estimated negligible at NLO).



Finite formulation $\implies$ further approximations only in $\mathrm{Re}\left\langle \mathcal{R}_0^{(0)} \middle| \mathcal{R}_0^{(2)} \right\rangle$.

No approximations in log-enhanced terms (very important!)

Computational setup

Implementation

Implementation

- Extension of MiNNLO$_{\text{PS}}$ to $Q\bar{Q}+F$ processes implemented within POWHEG-BOX-RES
- Some contributions to $\mathbf{D}$ evaluated by numerical integration (requires some care!) [Devoto, Mazzitelli, in preparation]
- Pythia for QCD,QED showers, MPI, hadronization
- OpenLoops for tree and one-loop amplitudes, including color- and spin-correlated

Massless two-loop corrections

Numerical code based on analytic results [Abreu, Febres Cordero, Ita, Klinkert, Page, VS '21], one-mass pentagon functions in `PentagonFunctions++` [Chicherin, VS, Zoia '21]

⚠ Challenging numerics: huge expressions $\mathcal{O}(1\text{Gb}) \implies$ high memory usage, elaborate numerical stability checks and rescue through higher precision

- Noticeable fraction of total CPU time for two-loop contributions

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SOON: new "simplified" analytic form [de Laurentis, Ita, Page, VS, in preparation]: $17\times$ faster, $11\times$ less memory

Phenomenology

Inclusive cross sections

	σ_{total} [pb]	ratio to NLO
NLO+PS	$32.21(0)^{+16.4\%}_{-13.4\%}$	1.000
MiNLO′	$22.33(1)^{+28.2\%}_{-17.9\%}$	0.693
MiNNLO$_{\text{PS}}$	$50.58(4)^{+16.8\%}_{-12.2\%}$	1.588

- $\sqrt{s} = 13$ TeV, $m_{\ell^+\ell^-} \in [67\,\text{GeV}, 116\,\text{GeV}]$
- Main Born scale $\mu_R = m_{b\bar{b}\ell\ell}$
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- $\log m_b$-enhanced contributions from closed b loops small (larger in CMS fiducial region)

Comparison to CMS measurement

Compare to CMS $\sqrt{s} = 13\,\text{TeV}$ complete Run 2 data [Phys. Rev. D 105 (2022) 092014]

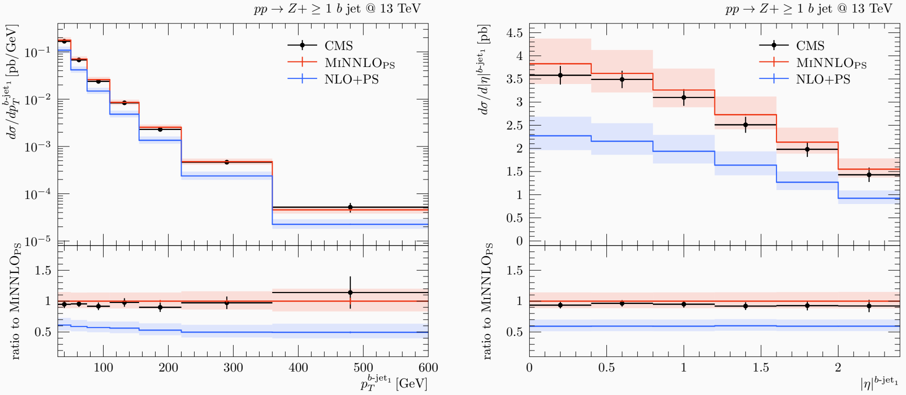
- Unfolded to fiducial region
- Backgrounds ($t\bar{t}, Z+$ jets) subtracted by MC simulations

σ_{fiducial} [pb]	$Z+\geq 1$ b-jet	$Z+\geq 2$ b-jets
NLO+PS	4.08 ± 0.66	0.44 ± 0.08
MiNNLO$_{\text{PS}}$	6.72 ± 0.91	0.79 ± 0.10
NLO+PS (5FS) [CMS]	7.03 ± 0.47	0.77 ± 0.07
CMS	6.52 ± 0.43	0.65 ± 0.08

- Hadronization, MPI included
- Apply experimental definition of b-jets (at the level of hadrons)

- Tension between NLO+PS(4FS) and data lifted upon inclusion of NNLO
- Excellent agreement between MiNNLO$_{\text{PS}}$ and NLO+PS(5FS)

Differential distributions: 1-b-jet



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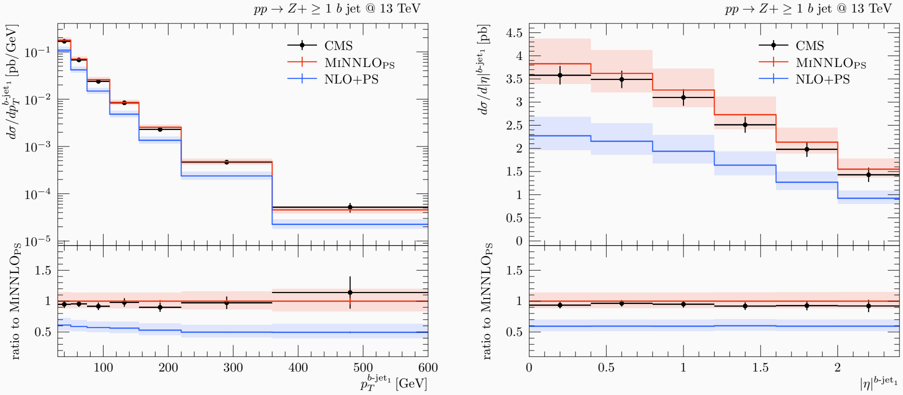
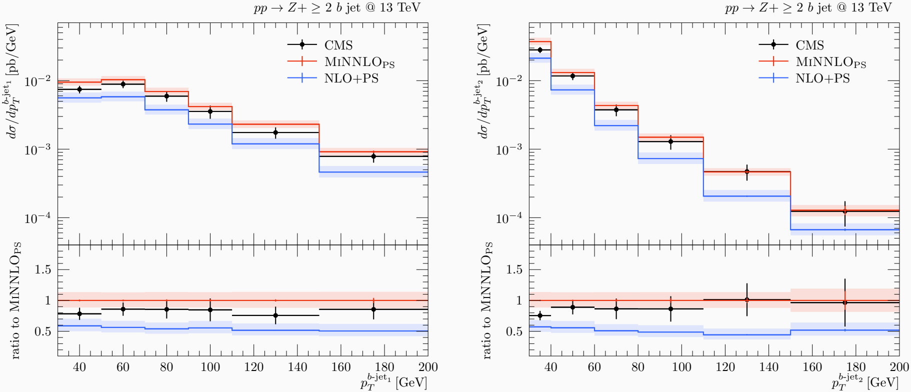


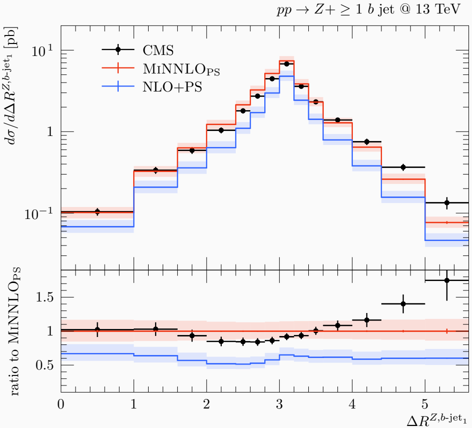
- NLO+PS fails to describe normalization
- $p_T^{b\text{-jet}_1}$ shape significantly corrected
- MiNNLO$_{PS}$ predictions in remarkable agreement with data
- Theory uncertainty still larger than experimental in most bins

Differential distributions: 2-b-jet



- Normalization slightly higher than data
- Still MiNNLO$_{PS}$ predictions in good agreement with data (also seen in other 2-b-jet distributions)

Angular separation between Z boson and leading b-jet



- Data not described well at high $\Delta R^{Z,b_{\text{-jet}}}$

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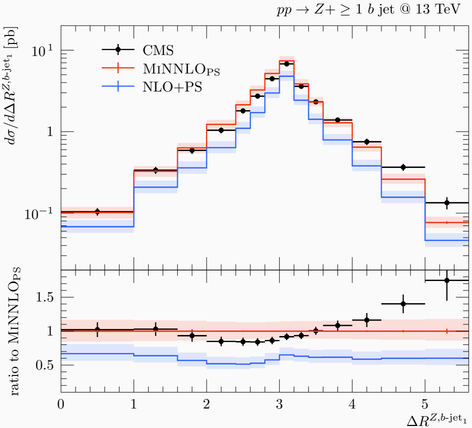

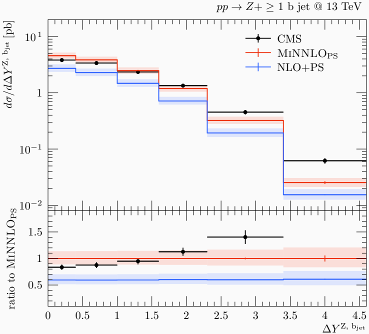

$$\Delta R = \sqrt{\Delta\phi^2 + \Delta\eta^2}$$

- Data not described well at high $\Delta R^{Z,b\text{-jet}}$
- Traced to $\Delta Y^{Z,b\text{-jet}_1}$
- Resummation of m_b logs (5FS) especially important?

Conclusions & Outlook

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Outlook

- Detailed comparison to fixed order NNLO predictions [Work in progress]
- Comparison to NNLO 5FS predictions (b jets!)
- Careful study of PS and MPI effects
- Significantly improved implementation of two-loop corrections
  [de Laurentis, Ita, Page, VS, in preparation]
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Thank you for your attention! Stay tuned!

Acknowledgments

This work has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme grant agreement 101019620 (ERC Advanced Grant TOPUP).

European Research Council

Established by the European Commission

Backup

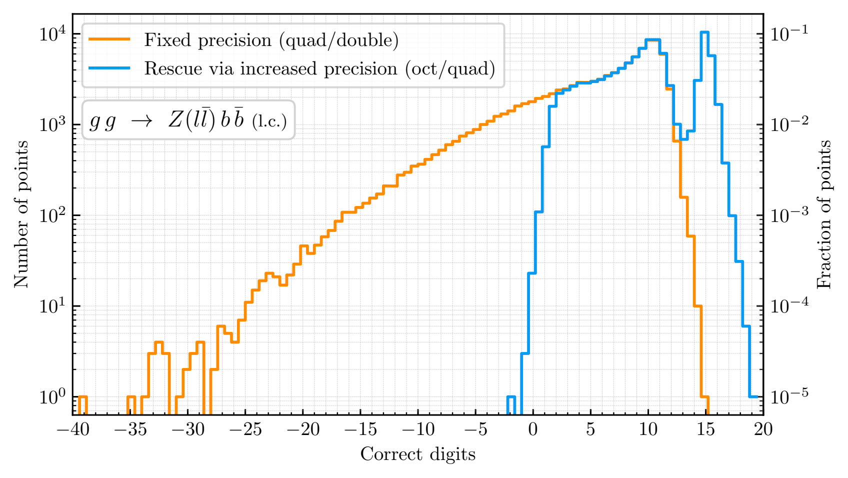
CMS fiducial region

[arXiv:2112.09659]
Final state: $Z \to \ell^+\ell^-$ (electrons or muons), and at least one (or two) b-jets.

- $71\,\mathrm{GeV} \leq m_{\ell^+\ell^-} \leq 111\,\mathrm{GeV}$
- Lepton selection: $p_T^\ell > 25$ GeV, $p_T^{\ell_1} > 35$ GeV, $|\eta^\ell| < 2.4$
- Events with more than two leptons vetoed
- Leptons "dressed" by adding the momenta of all photons within $\Delta R^{\gamma,\ell} \leq 0.1$
- Anti-k_T b-jets with $R = 0.4$, $p_T^{b\text{-jet}} > 30\,$GeV and $|\eta^{b\text{-jet}}| < 2.4$
- b tagged if at least one b-flavored hadron in the jet
- Overlap between leptons and b-jets vetoed: $\Delta R^{\ell,b\text{-jet}} > 0.4$

Two-loop numerical stability

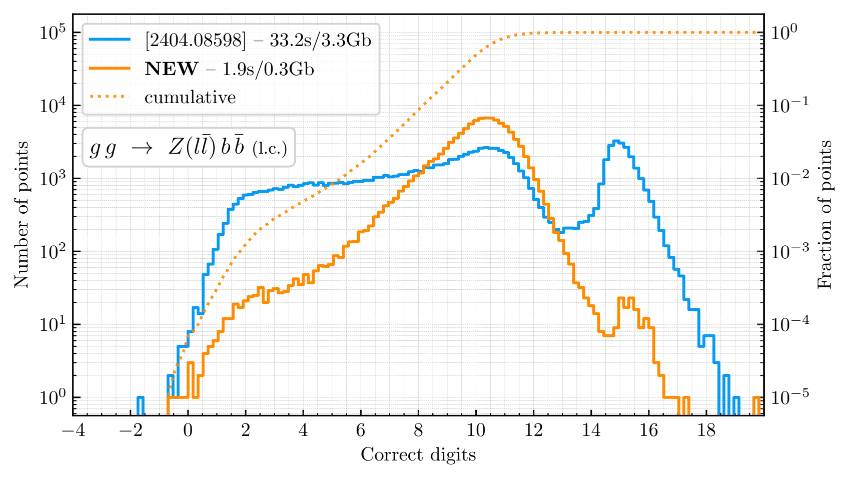
- Learn to detect unstable points very well, switch to higher precision dynamically.



New analytic representation

New analytic representation after basis change and iterated pole subtractions

[de Laurentis, Ita, Page, VS in preparation]



100% Eco Friendly

- Significantly improved stability.
- 17 times faster evaluations, 11 times less memory.