MC@NLO-Δ
and statistical fluctuations at fixed order

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Outline

- NLO+PS: MC@NLO-Δ
  - Together with S. Frixione, S. Prestel and P. Torrielli, 2002.12716 [hep-ph] and with Pythia8 support from L. Gellersen and C. Preuss

- Applications for fixed order

MC@NLO-Δ

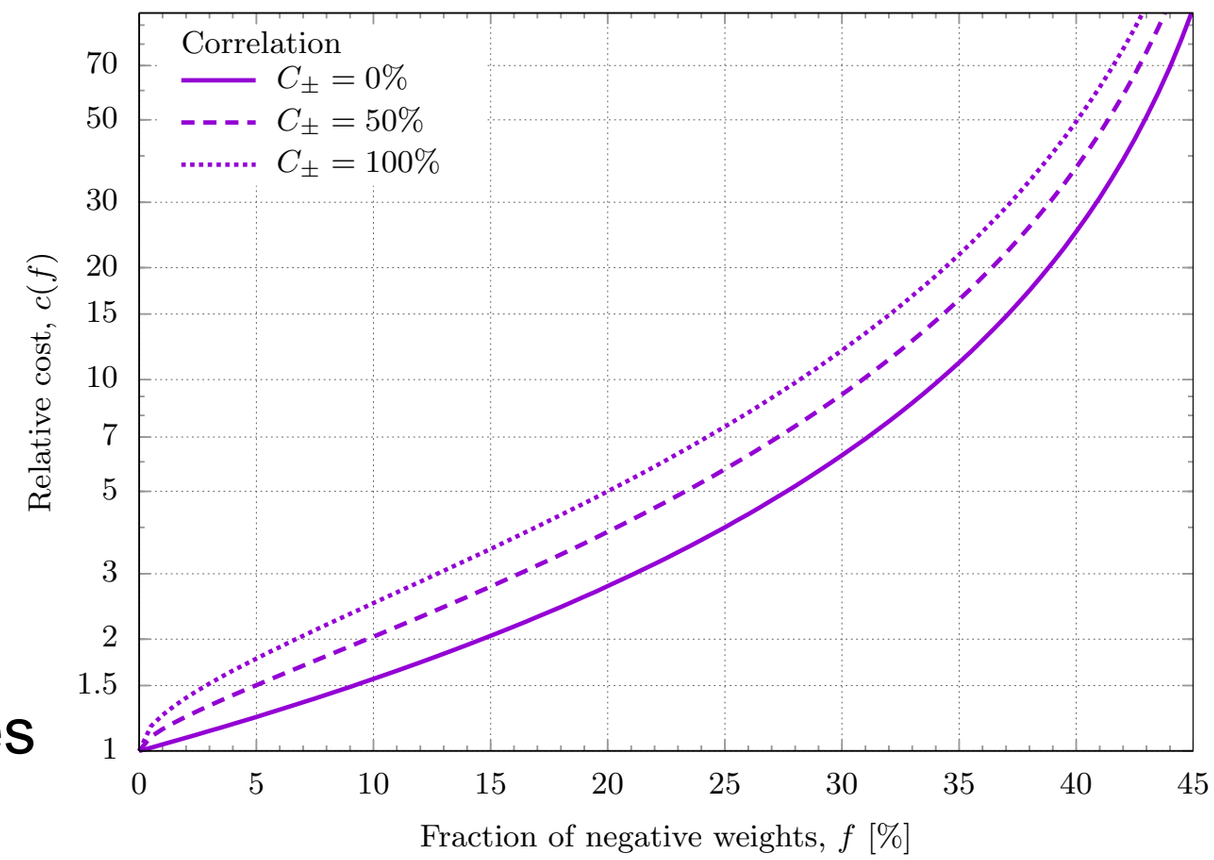
The cost of negative weights

- Main disadvantage of MC@NLO is the (large) fraction of negatively weighted events
  - IR-safe observables will be positive in all bins
    (up to statistical fluctuations)
- Efficiency and relative cost:

$$\varepsilon(f) = 1 - 2f$$

$$c(f) = \frac{1 + C_{\pm}\sqrt{1 - \varepsilon(f)^2}}{\varepsilon(f)^2}$$

- Not only is there a cancelation between negative and positive events, the remaining distributions still have the statistical uncertainties of the original (larger) event files



MC@NLO anatomy

- Generating functional for MC@NLO

$$\mathcal{F}_{\mathrm{MC@NLO}} = \mathcal{F}_{\mathrm{MC}}\left(\mathcal{K}^{(\mathbb{H})}\right) d\sigma^{(\mathbb{H})} + \mathcal{F}_{\mathrm{MC}}\left(\mathcal{K}^{(\mathbb{S})}\right) d\sigma^{(\mathbb{S})}$$

MC (Shower) functional, starting from (n+1)-body kinematics

MC (Shower) functional, starting from n-body kinematics

with

real emission

shower counter terms

H-events: $d\sigma^{(\mathbb{H})} = d\sigma^{(\mathrm{NLO},E)} - d\sigma^{(\mathrm{MC})}$,

S-events: $d\sigma^{(\mathbb{S})} = d\sigma^{(\mathrm{MC})} + \sum_{\alpha=S,C,SC} d\sigma^{(\mathrm{NLO},\alpha)}$

Born, virtual, soft/collinear

MC@NLO
origins of negative weights

$$\mathcal{F}_{\mathrm{MC@NLO}} = \mathcal{F}_{\mathrm{MC}}\left(\mathcal{K}^{(\mathbb{H})}\right) d\sigma^{(\mathbb{H})} + \mathcal{F}_{\mathrm{MC}}\left(\mathcal{K}^{(\mathbb{S})}\right) d\sigma^{(\mathbb{S})}$$

$$d\sigma^{(\mathbb{H})} = d\sigma^{(\mathrm{NLO},E)} - d\sigma^{(\mathrm{MC})},$$

$$d\sigma^{(\mathbb{S})} = d\sigma^{(\mathrm{MC})} + \sum_{\alpha=S,C,SC} d\sigma^{(\mathrm{NLO},\alpha)}$$

- Three sources of negative weights (with some overlap in the first two)

N.1 $\mathbb{H}$ events with $P(\mathcal{K}^{(\mathbb{H})}) \ll M_H$;

N.2 $\mathbb{H}$ events with $P(\mathcal{K}^{(\mathbb{H})}) \sim M_H$;

Shower counter terms overestimate the real-emission corrections

N.3 $\mathbb{S}$ events.

n-body kinematics, but support in n+1-body phase space

Types N.2 and N.3

N.1 $\mathbb{H}$ events with $P(\mathcal{K}^{(\mathbb{H})}) \ll M_H$;

N.2 $\mathbb{H}$ events with $P(\mathcal{K}^{(\mathbb{H})}) \sim M_H$;

N.3 $\mathbb{S}$ events.

$$\mathcal{F}_{\mathrm{MC@NLO}} = \mathcal{F}_{\mathrm{MC}}\left(\mathcal{K}^{(\mathbb{H})}\right) d\sigma^{(\mathbb{H})} + \mathcal{F}_{\mathrm{MC}}\left(\mathcal{K}^{(\mathbb{S})}\right) d\sigma^{(\mathbb{S})}$$

$$d\sigma^{(\mathbb{H})} = d\sigma^{(\mathrm{NLO},E)} - d\sigma^{(\mathrm{MC})},$$

$$d\sigma^{(\mathbb{S})} = d\sigma^{(\mathrm{MC})} + \sum_{\alpha=S,C,SC} d\sigma^{(\mathrm{NLO},\alpha)}$$

- Reduction of negative events of type N.2
  - The shower is radiating into the hard region; fine for LO, but at NLO one emission is explicitly included through real-emission matrix elements
    $\Longrightarrow$ prefer smaller shower starting scales
- Reduction of negative events of type N.3
  - These are n-body contributions, but have support in (n+1)-body phase-space
    $\Longrightarrow$ sample +1-phase-space more often for a given n-body point
  - Identical to "folding" in the POWHEG codes

MC@NLO-Δ

N.1 $\mathbb{H}$ events with $P(\mathcal{K}^{(\mathbb{H})}) \ll M_H$;

N.2 $\mathbb{H}$ events with $P(\mathcal{K}^{(\mathbb{H})}) \sim M_H$;

N.3 $\mathbb{S}$ events.

$$\mathcal{F}_{\text{MC@NLO}} = \mathcal{F}_{\text{MC}}\left(\mathcal{K}^{(\mathbb{H})}\right) d\sigma^{(\mathbb{H})} + \mathcal{F}_{\text{MC}}\left(\mathcal{K}^{(\mathbb{S})}\right) d\sigma^{(\mathbb{S})}$$

$$d\sigma^{(\mathbb{H})} = d\sigma^{(\text{NLO},E)} - d\sigma^{(\text{MC})}\,,$$

$$d\sigma^{(\mathbb{S})} = d\sigma^{(\text{MC})} + \sum_{\alpha=S,C,SC} d\sigma^{(\text{NLO},\alpha)}$$

- Reduction of negative events of type N.1
  - Modify the MC@NLO procedure:

$$\mathcal{F}_{\text{MC@NLO-}\Delta} = \mathcal{F}_{\text{MC}}\left(\mathcal{K}^{(\mathbb{H})}\right) d\sigma^{(\Delta,\mathbb{H})} + \mathcal{F}_{\text{MC}}\left(\mathcal{K}^{(\mathbb{S})}\right) d\sigma^{(\Delta,\mathbb{S})}$$

$$d\sigma^{(\Delta,\mathbb{H})} = \left(d\sigma^{(\text{NLO},E)} - d\sigma^{(\text{MC})}\right)\Delta\,,$$

$$d\sigma^{(\Delta,\mathbb{S})} = d\sigma^{(\text{MC})}\Delta + \sum_{\alpha=S,C,SC} d\sigma^{(\text{NLO},\alpha)} + d\sigma^{(\text{NLO},E)}\left(1-\Delta\right)$$

  - with

    $\Delta \longrightarrow 0$ in the soft/collinear limits

    $\Delta \longrightarrow 1$ in the hard regions

    $\Longrightarrow$ use shower no-emission probability (between hard scale and scale of the emission)

NLO accuracy

- The formal expansion of the no-emission probability is
  $\Delta = 1 + \mathcal{O}(\alpha_S)$
- Furthermore, in the soft/collinear limits the logarithms are similar to the ones that are generated by the shower

  $\Longrightarrow$ From this one can conclude that accuracy is the same as with the default MC@NLO method

- However, beyond NLO contributions can be very much different: MC@NLO-Δ is effectively a new matching procedure

Implementation

- Run-time interface between MG5_aMC and Pythia8
  - MG5_aMC generates a phase-space points, all the relevant matrix elements and MC counter terms
  - It calls Pythia8 to determine the relevant emission scales for each dipole in the S-events to obtain the H-event
  - For fast evaluation, the Pythia8 Sudakov factors have been tabulated (2D grids (dipole mass and scale); one for each parton flavour; one for each dipole type (II, IF, FI, FF))
  - No emission probabilities included by MG5_aMC
- Major complication:
  - emission scale is different for each dipole
  - when showering events requires a different starting scale for each dipole

MG5_aMC public version?

- Published MC@NLO-Δ in 2002.12716 [hep-ph], but code not yet public…
  - After publication, we found
    - some bugs…
    - a better treatment of events that are in the dead zone
    - some improvements in the shower scale assignments
    - compatibility with Pythia8.3
      (thanks to Leif Gellersen and Christian Preuss!)
  - Code will go public soon!

Reduction of negative weights

	MC@NLO			MC@NLO-Δ		
	111	212	414	111-Δ	212-Δ	414-Δ
$pp \to e^+e^-$	7.1% (1.4)	3.6% (1.2)	3.3% (1.1)	5.7% (1.3)	2.9% (1.1)	2.8% (1.1)
$pp \to e^+\nu_e$	7.3% (1.4)	4.0% (1.2)	3.7% (1.2)	6.1% (1.3)	3.5% (1.2)	3.3% (1.1)
$pp \to h$	10.4% (1.6)	4.8% (1.2)	3.4% (1.2)	4.2% (1.2)	1.3% (1.1)	0.4% (1.0)
$pp \to t\bar{t}$	22.9% (3.4)	20.0% (2.8)	19.5% (2.7)	10.1% (1.6)	5.1% (1.2)	4.4% (1.2)
$pp \to W^+t\bar{t}$	16.0% (2.2)	15.0% (2.0)	15.2% (2.1)	11.6% (1.7)	10.4% (1.6)	10.2% (1.6)
$pp \to hb\bar{b}$	40.1% (25.7)	37.9% (17.1)	37.4% (15.7)	36.7% (14.2)	31.2% (7.0)	29.9% (6.2)
$pp \to W^+j[50]$	21.7% (3.1)	16.3% (2.2)	15.7% (2.1)	15.4% (2.1)	7.7% (1.4)	6.0% (1.3)

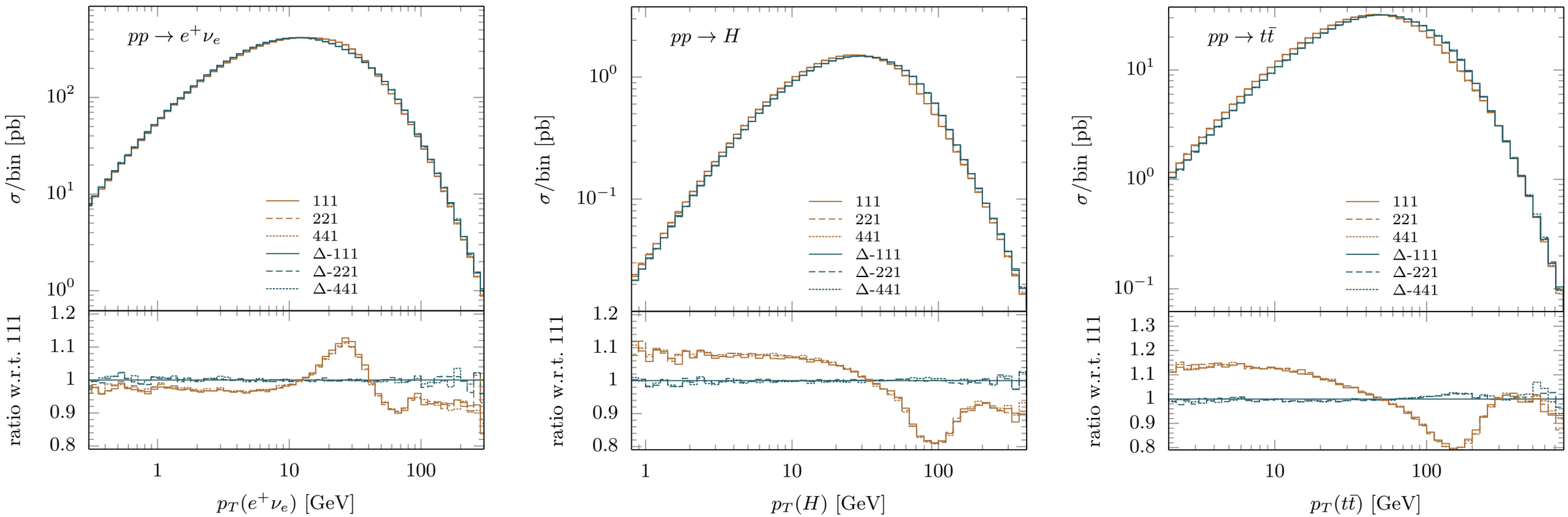
no folding

4x folding

16x folding

- Fraction of negative weights and relative cost (assuming no correlations)

Selected results



- Transverse momentum of the Born system
- Differences between default and Δ are sizeable, but reasonable
- Folding has no effect (apart from increased statistics), as it should be

Summary, part 1

- MC@NLO-Δ reduces the number of negative weights by a significant amount
  - New matching procedure; results differ from default MC@NLO—within the matching systematics
  - Run-time interface between MG5_aMC and Pythia8
    - With Δ enabled, CPU time to generate LHEF increases by a factor ~3
    - 4x folding increases the run time also by a factor ~3
    - 16x folding about a factor ~3^2

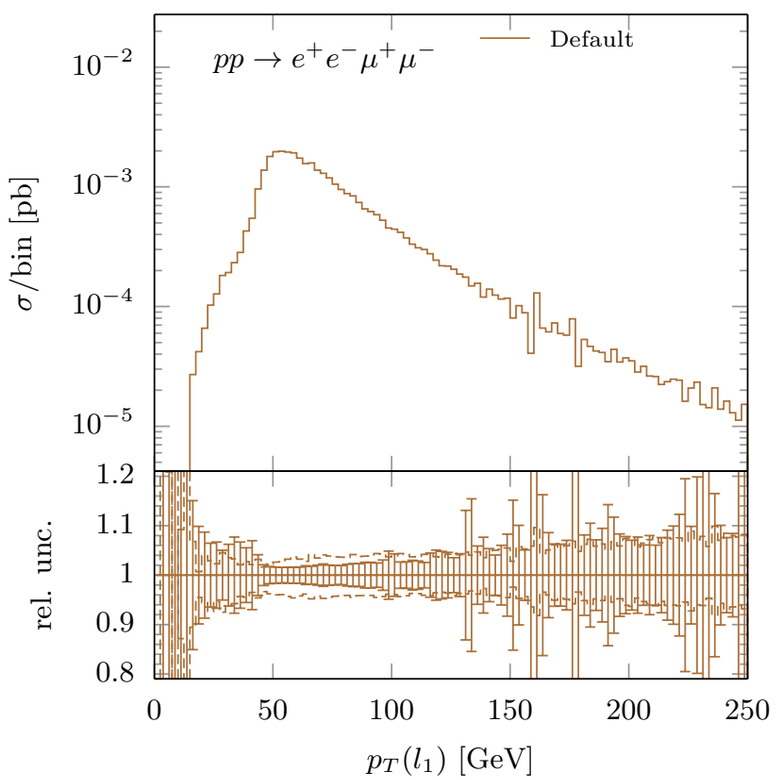
    ⟹ reduction of negative weights due to Δ and folding typically not worth it from a CPU point of view, except when there is more overhead than simply showering the events (detector simulation, storage space, etc.)

- Outlook: multi-jet FxFx merging within MC@NLO-Δ is the next step

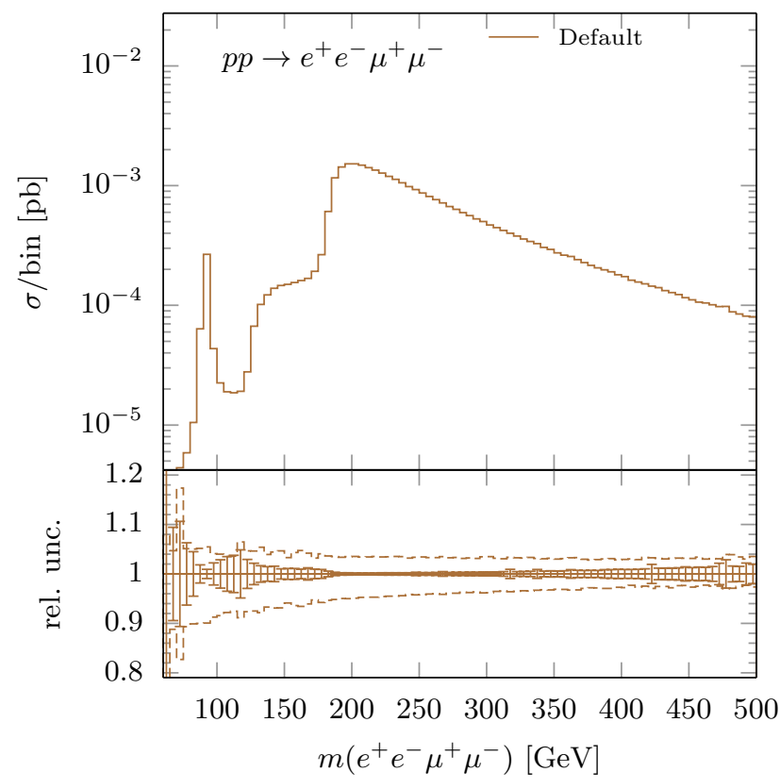
Reducing statistical fluctuations at Fixed Order

Statistical fluctuations at fixed order

- A major source of statistical fluctuations in fixed order differential distributions are the 'misbinning' effects
  - At NLO: the real-emission and IR-subtraction terms can end up in different bins
  - This depends on the mapping between the n and (n+1)-body phase-space



large statistical fluctuations for lepton p_T's



no misbinning for e.g. 4-lepton invariant mass

Δ for Fixed order

- NLO diff. cross section (schematically)

$$\frac{d\sigma^{\mathrm{NLO}}}{d\mathcal{O}} = \int (B+V+I)\mathcal{O}(\Phi_n)\, d\Phi_n + \int (R\mathcal{O}(\Phi_{n+1}) - S\mathcal{O}(\Phi_n))\, d\Phi_{n+1}$$

- Introduce Δ factor:

$$\frac{d\sigma^{\mathrm{NLO}}}{d\mathcal{O}} = \int (B+V+I)\mathcal{O}(\Phi_n)\, d\Phi_n + \int \Big[(R\mathcal{O}(\Phi_{n+1}) - R\mathcal{O}(\Phi_n))\Delta + R\mathcal{O}(\Phi_n) - S\mathcal{O}(\Phi_n) \Big]\, d\Phi_{n+1}$$

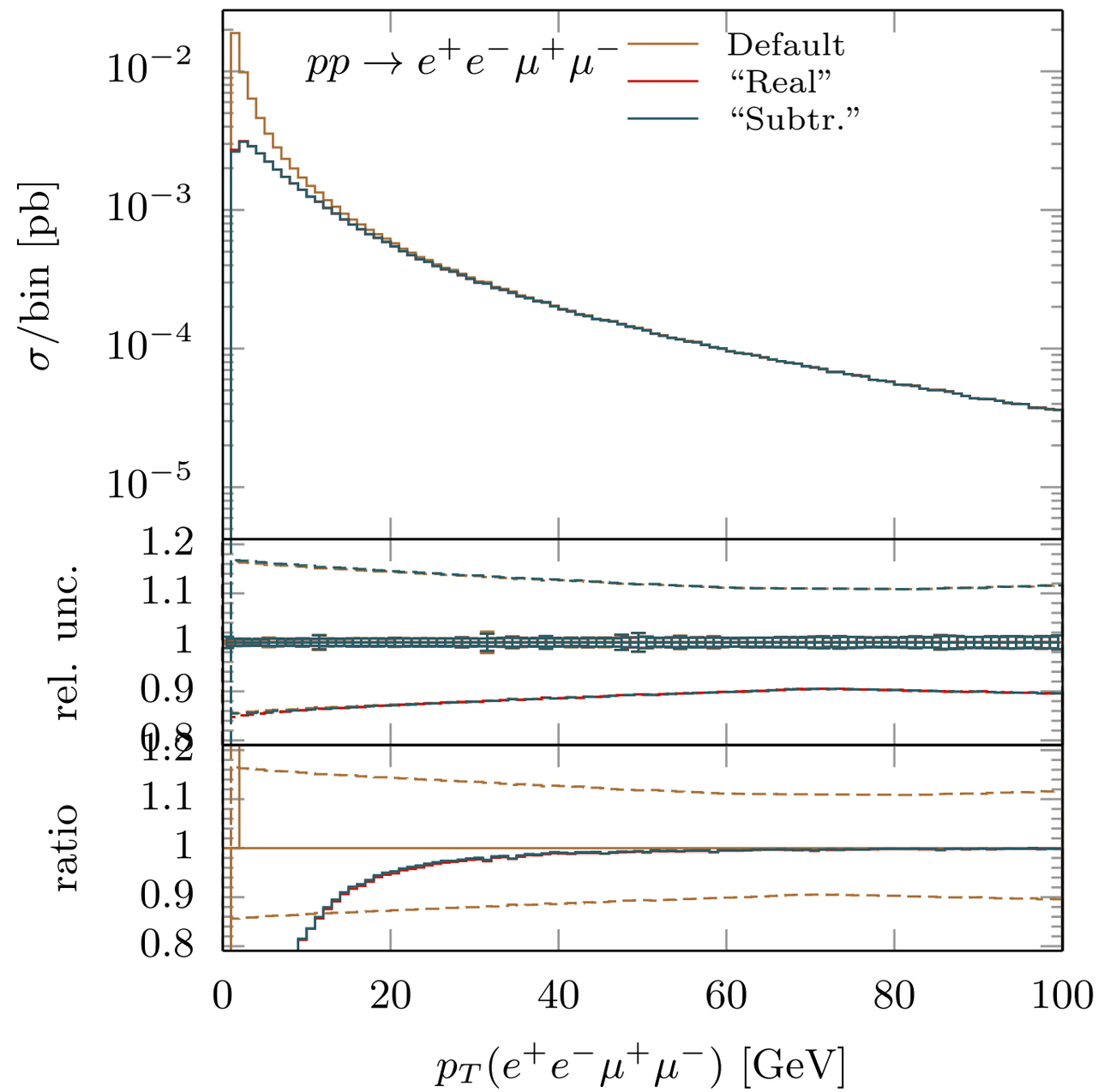
Alternatively:

$$\frac{d\sigma^{\mathrm{NLO}}}{d\mathcal{O}} = \int (B+V+I)\mathcal{O}(\Phi_n)\, d\Phi_n + \int \Big[R\mathcal{O}(\Phi_{n+1}) - S\mathcal{O}(\Phi_{n+1}) + (S\mathcal{O}(\Phi_{n+1}) - S\mathcal{O}(\Phi_n))\Delta \Big]\, d\Phi_{n+1}$$

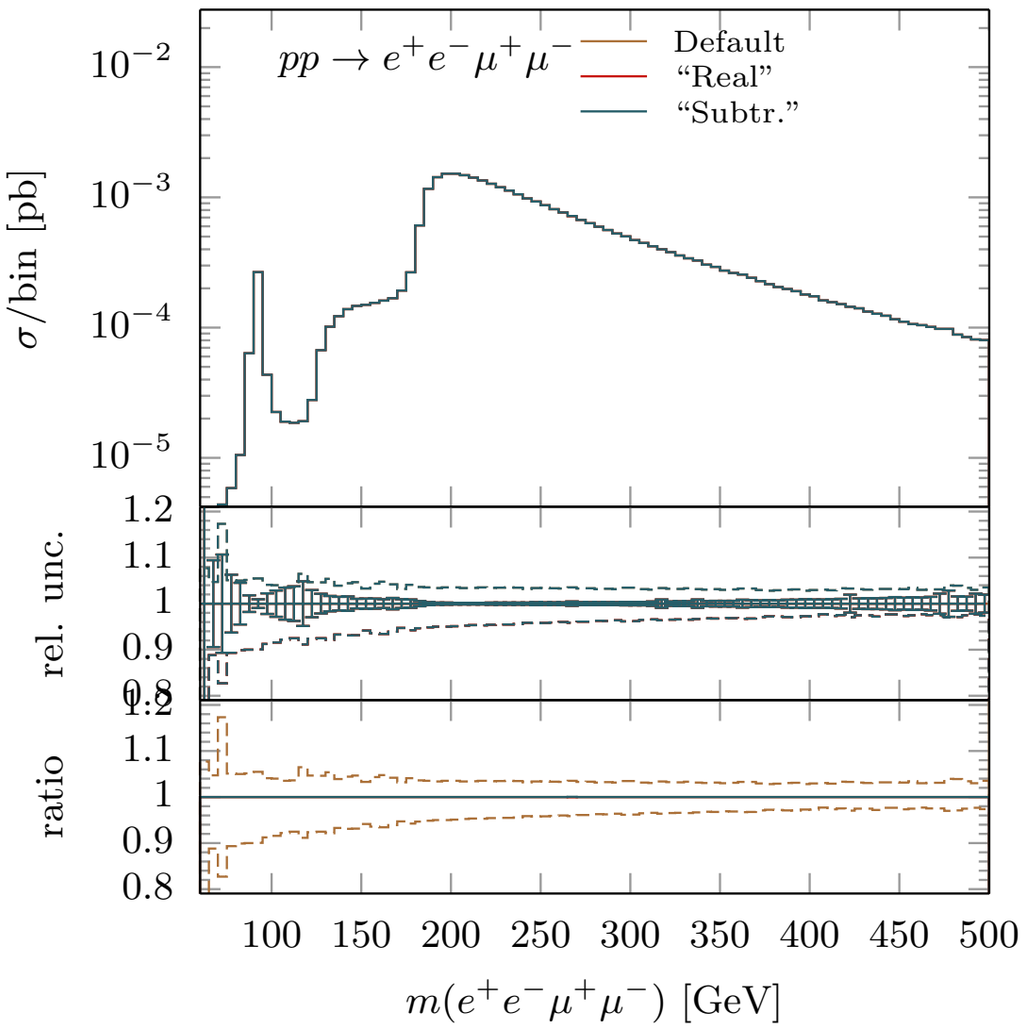
- Δ does not need to be the Pythia8 no-emission probability: it can be a simple LL Sudakov factor between the hard scale and the scale of the emission
  $\Longrightarrow$ NLO accuracy is conserved

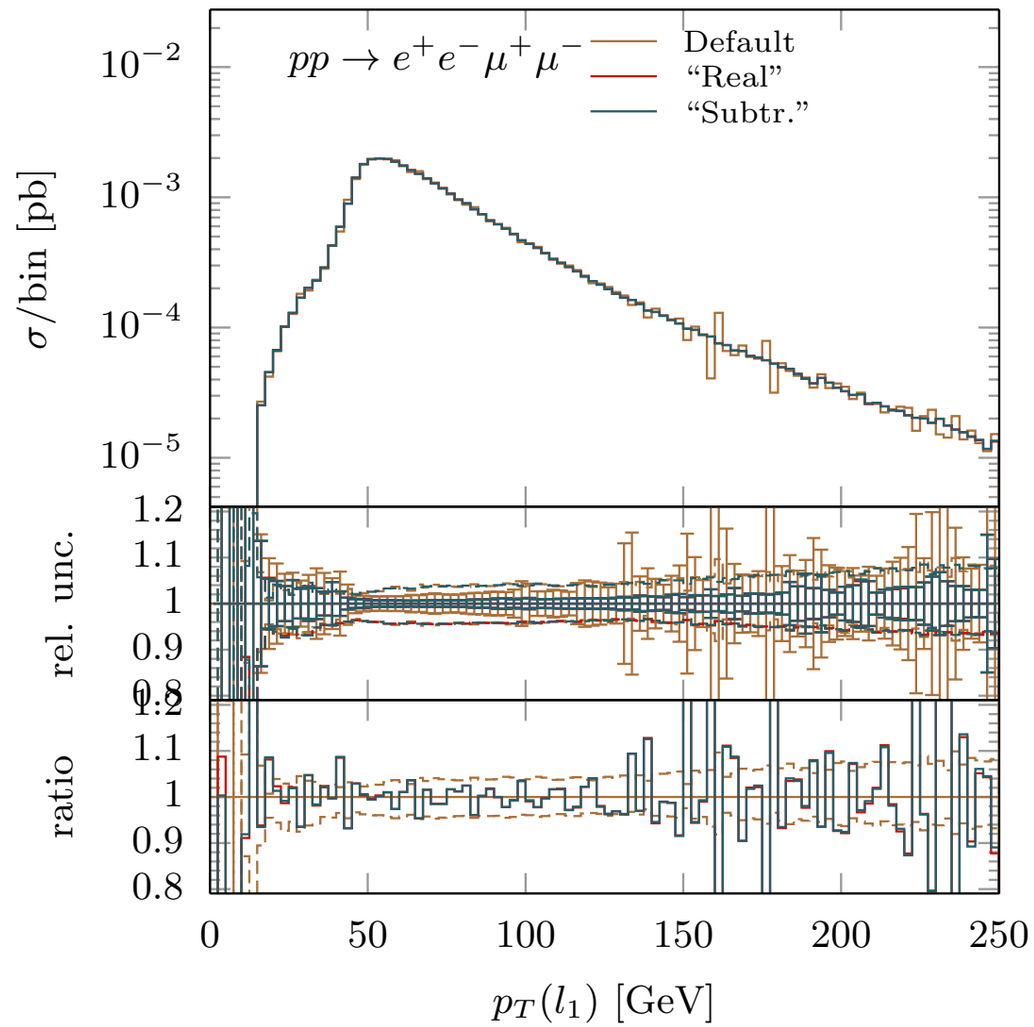
p_T(4lepton)

- Same random seed: exactly the same PS points
- Inclusion of Δ changes the 4-lepton spectrum at small transverse momenta
- However, this is the region where you cannot trust FO perturbation theory
- Two versions (including Δ for real and subtraction, respectively) give identical results



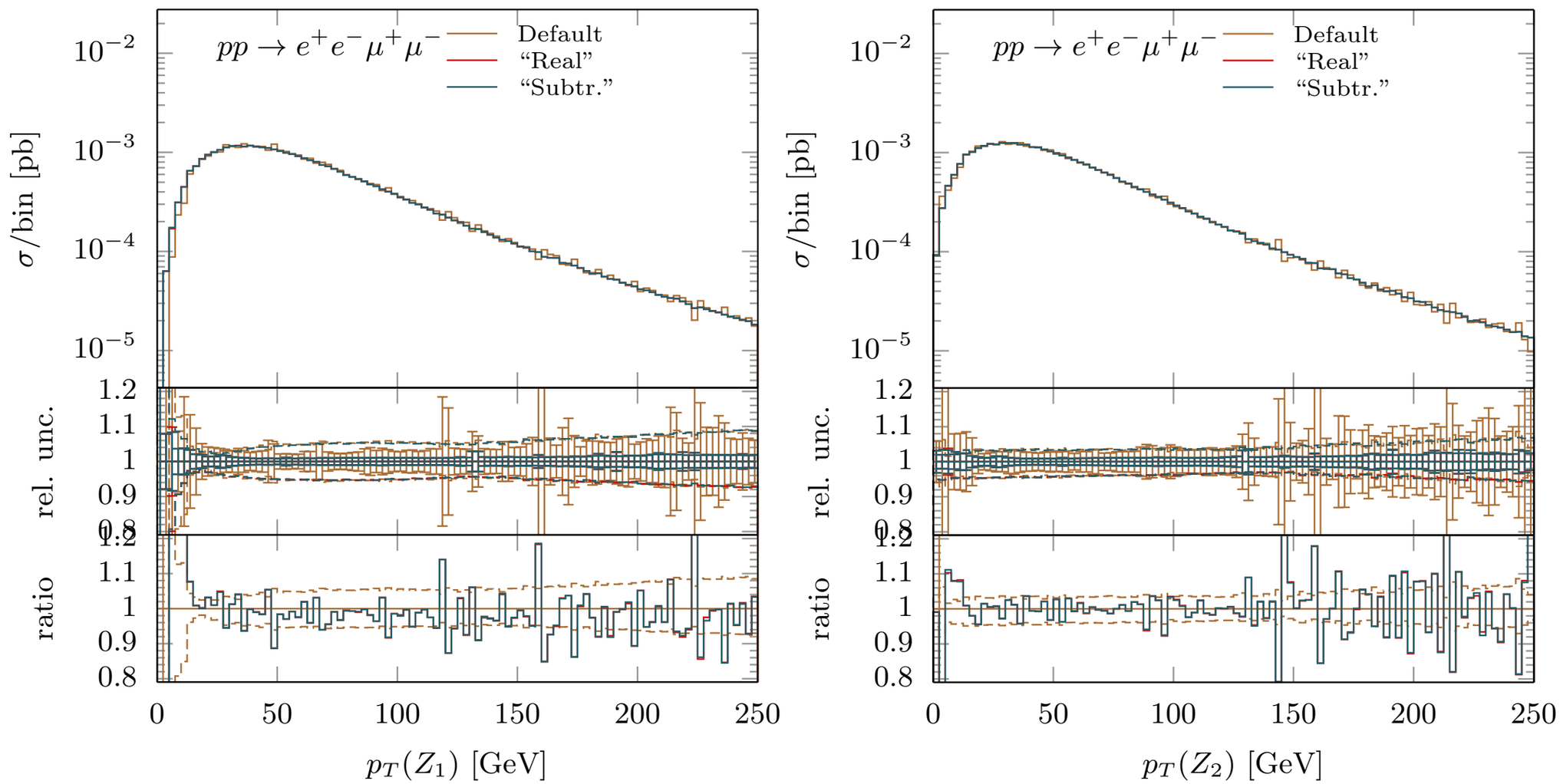
Hardest lepton and invariant mass





- Of course, no effect in 4-lepton invariant mass
- Significant reduction of statistical fluctuations in $p_T(l_1)$; compatible with the default

Z-bosons (ordered in p_T)



- Again, large reduction in statistical fluctuations
- Compatible within scale uncertainties;
  expect at low $p_T(Z)$, where FO perturbation theory cannot be trusted

Summary, part 2

- Adding Δ is a simple improvement to fixed order computations that can significantly reduce statistical fluctuations in diff. distributions
- Inclusive rates are not affected
  $\Longrightarrow$ Observables conserved in the mapping are not affected
- Other observables see some changes, but only when sensitive to IR region, where fixed order perturbation theory does not work
  $\Longrightarrow$ Statistical fluctuations reduced by factor ~2-3 at no additional cost. Severe misbinning is gone
- Worth investigating for other processes and at NNLO