Numerical challenges in NNLO slicing

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NLO QCD cross section via dipole subtraction

Schematic formula for the NLO cross section with dipoles [Catani, Seymour (1993), Catani, Dittmaier, Seymour, Trocsanyi (2002)]

$$\delta\sigma^{\mathrm{NLO}} = \underbrace{\int_{m+1} d\sigma^R}_{\text{real}} + \underbrace{\int_m d\sigma^V}_{\text{virtual}} + \underbrace{\int_0^1 dz \int_m d\sigma^C}_{\text{collinear}} - \int_{m+1} d\sigma^A + \int_{m+1} d\sigma^A$$

$$d\sigma^A = \sum_{\text{dipoles}} d\sigma^B \otimes dV_{\text{dipole}} \qquad \int_1 dV_{\text{dipole}} = \int dz \Big([dV_{\text{dipole}}(z)]_+ + V_{\text{dipole}}(1)\delta(1-z) \Big)$$

$$= \underbrace{\int_{m+1} \Big[d\sigma^R - \sum_{\text{dipoles}} d\sigma^B \otimes dV_{\text{dipole}} \Big]_{\epsilon=0}}_{\text{subtracted real} \;\Rightarrow\; \boldsymbol{\delta\sigma^{\mathrm{RA}}}} + \underbrace{\int_m \Big[d\sigma^V + \sum_{\text{dipoles}} d\sigma^B \otimes V_{\text{dipole}}(1) \Big]_{\epsilon=0}}_{\text{virtual} + I\text{-operator} \;\Rightarrow\; \boldsymbol{\delta\sigma^{\mathrm{VA}}}}$$

$$+ \underbrace{\int_0^1 dz \int_m \Big[d\sigma^C + \sum_{\text{dipoles}} d\sigma^B(z) \otimes [dV_{\text{dipole}}(z)]_+ \Big]_{\epsilon=0}}_{K+P \text{ terms} \;\Rightarrow\; \boldsymbol{\delta\sigma^{\mathrm{CA}}}}$$

➥ **Local subtraction terms** mediate **infrared (soft and collinear) divergences** between phase spaces

Idea of the q_{T} subtraction method for (N)NLO cross sections

Consider the production of a **colourless final state F** via $\mathrm{q\bar{q}} \to \mathbf{F}$ or $\mathrm{gg} \to \mathbf{F}$: $\mathbf{d}\boldsymbol{\sigma}_{\mathbf{F}}^{\mathbf{(N)NLO}}\Big|_{q_{\mathrm{T}}\neq 0} = \mathbf{d}\boldsymbol{\sigma}_{\mathbf{F+jet}}^{\mathbf{(N)LO}}$
where q_{T} refers to the transverse momentum of the colourless system F [Catani, Grazzini (2007)]

- $\mathbf{d}\boldsymbol{\sigma}_{\mathbf{F}}^{\mathbf{(N)NLO}}\Big|_{q_{\mathrm{T}}\neq 0}$ is singular for $q_{\mathrm{T}} \to 0$
  - ➥ limiting behaviour known from transverse-momentum resummation [Bozzi, Catani, de Florian, Grazzini (2006)]
- Define a universal counterterm $\boldsymbol{\Sigma}$ with the complementary $q_{\mathrm{T}} \to 0$ behaviour [Bozzi, Catani, de Florian, Grazzini (2006)]
  $\mathbf{d}\boldsymbol{\sigma}^{\mathbf{CT}} = \boldsymbol{\Sigma}(q_{\mathrm{T}}/q) \otimes \mathbf{d}\boldsymbol{\sigma}^{\mathbf{LO}}$ where q is the invariant mass of the colourless system F
- Add the $q_{\mathrm{T}} = 0$ piece with the hard–virtual coefficient $\mathcal{H}_{\mathrm{F}}$, which contains the 1-(2-)loop amplitudes at (N)NLO and compensates for the subtraction of $\boldsymbol{\Sigma}$ [Catani, Cieri, de Florian, Ferrera, Grazzini (2013)]

➥ **Master formula for (N)NLO cross section in q_{T} subtraction method**

$$\mathbf{d}\boldsymbol{\sigma}_{\mathbf{F}}^{\mathbf{(N)NLO}} = \mathcal{H}_{\mathbf{F}}^{\mathbf{(N)NLO}} \otimes \mathbf{d}\boldsymbol{\sigma}^{\mathbf{LO}} + \left[\mathbf{d}\boldsymbol{\sigma}_{\mathbf{F+jet}}^{\mathbf{(N)LO}} - \boldsymbol{\Sigma}^{\mathbf{(N)NLO}} \otimes \mathbf{d}\boldsymbol{\sigma}^{\mathbf{LO}}\right]_{\mathrm{cut}_{q_{\mathrm{T}}/q}\to 0}$$

- all ingredients known for extension to N^{3}LO [Luo, Yang, Zhu, Zhu (2019; 2020), Ebert, Mistlberger, Vita (2020), Cieri, Chen, Gehrmann, Glover, Huss (2019), Camarda, Cieri, Ferrera (2021), Chen, Gehrmann, Glover, Huss, Yang, Zhu (2021)]

Extension to heavy coloured particles at NNLO QCD and beyond

Extension of q_T subtraction method to production of heavy coloured particles ($Q\bar{Q}$, $Q\bar{Q}X$, etc.)

$$d\sigma^{\mathrm{NNLO}}_{Q\bar{Q}X} = \mathcal{H}^{\mathrm{NNLO}}_{Q\bar{Q}X} \otimes d\sigma_{\mathrm{LO}} + \left[d\sigma^{\mathrm{NLO}}_{Q\bar{Q}X+\mathrm{jet}} - d\sigma^{\mathrm{NNLO}}_{Q\bar{Q}X,\mathrm{CT}} \right]_{\mathrm{cut}_{q_T/q}\to 0}$$

- counterterm accounts for IR behaviour of real contribution, including soft singularities related to emissions from final-state quarks [Catani, Grazzini, Torre (2014), Ferroglia, Neubert, Pecjak, Yang (2009), Li, Li, Shao, Yang, Zu (2013), Catani, Grazzini, Fabre, SK (2021)]
- massive NLO subtraction required for real-emission part, e.g. massive dipole subtraction [Catani, Seymour (1997), Catani, Dittmaier, Seymour, Trocsanyi (2002)]
- $\mathcal{H}^{Q\bar{Q}X}_{\mathrm{NNLO}}$ contains remainder of integrated final-state soft singularities
  - known for heavy-quark pairs [Catani, Devoto, Grazzini, Mazzitelli (2023), Angeles-Martinez, Czakon, Sapeta (2018)]
  - more involved kinematics for associated heavy-quark pair production [Devoto, Mazzitelli (to appear)]

➥ talk by Simone Devoto

Extension of q_T subtraction method to mixed QCD–EW corrections of $\mathcal{O}(\alpha_s^m \alpha^n)$

$$d\sigma^{(m,n)}_{\mathrm{F}} = \mathcal{H}^{(m,n)}_{\mathrm{F}} \otimes d\sigma_{\mathrm{LO}} + \left[d\sigma^{(m,n)}_{\mathrm{F,R}} - d\sigma^{(m,n)}_{\mathrm{F,CT}} \right]_{\mathrm{cut}_{q_T/q}\to 0}$$

- limitation: F contains no massless jets (for $m \geq 1$) and no massless charged particles (for $n \geq 1$) [Buonocore, Grazzini, Tramontano (2020), Buonocore (2020), De Florian, Der, Fabre (2018), Cieri, De Florian, Der, Mazzitelli (2020)]

NLO QCD cross section via q_{T} subtraction

Schematic formula for the NLO cross section via q_{T} subtraction [Catani, Grazzini (2007)]

$$\delta\sigma^{\mathrm{NLO}} = \underbrace{\int_{m+1} d\sigma^R}_{\text{real}} + \underbrace{\int_m d\sigma^V}_{\text{virtual}} + \underbrace{\int_0^1 dz \int_m d\sigma^C}_{\text{collinear}}$$

$$= \underbrace{\int_{m+1} d\sigma^R\Big|_{q_{\mathrm{T}}/q\,>\,\mathrm{cut}_{q_{\mathrm{T}}/q}}}_{\substack{\text{integrated exactly over the}\\ m+1\text{ particle phase space}}} + \underbrace{\int_{m+1} d\sigma^R\Big|_{q_{\mathrm{T}}/q\,\leq\,\mathrm{cut}_{q_{\mathrm{T}}/q}}}_{\substack{\text{approximated by results known}\\ \text{from } q_{\mathrm{T}} \text{ resummation}}} + \underbrace{\int_m d\sigma^V + \int_0^1 dz \int_m d\sigma^C}_{\substack{\text{identified with corresponding terms}\\ \text{in } q_{\mathrm{T}} \text{ resummation}}}$$

$$\approx \underbrace{\int_{m+1} d\sigma^R\Big|_{q_{\mathrm{T}}/q\,>\,\mathrm{cut}_{q_{\mathrm{T}}/q}}}_{\substack{\text{finite tree-level contribution (F+jet),}\\ \text{explicit } \mathrm{cut}_{q_{\mathrm{T}}/q} \text{ dependence}}} + \underbrace{\int_0^1 dz \int_m \frac{\alpha_S}{\pi} \int_{\mathrm{cut}_{q_{\mathrm{T}}/q}}^{\infty} d(q_{\mathrm{T}}/q)\, \boldsymbol{\Sigma}^{(1)}(q_{\mathrm{T}}/q) \otimes d\sigma_{\mathrm{LO}}}_{\substack{\text{assigned to Born phase-space (without recoil),}\\ \text{implicit } \mathrm{cut}_{q_{\mathrm{T}}/q} \text{ dependence}}} + \underbrace{\int_0^1 dz \int_m \frac{\alpha_S}{\pi} \mathcal{H}_F^{(1)} \otimes d\sigma_{\mathrm{LO}}}_{\substack{\text{contains (finite) 1-loop part,}\\ \text{no } \mathrm{cut}_{q_{\mathrm{T}}/q} \text{ dependence}}}$$

➥ $\boldsymbol{\delta\sigma}^{\mathrm{RT}}$ ➥ $\boldsymbol{\delta\sigma}^{\mathrm{CT}}$ ➥ $\boldsymbol{\delta\sigma}^{\mathrm{VT}}$

➥ **Non-local q_{T} subtraction** mediates **infrared (soft and collinear) divergences** between phase spaces through a **slicing cut on q_{T}/q** ➥ cancellation happens only on the integrated level

NNLO QCD cross section via q_{T} subtraction

Schematic formula for the NNLO cross section via q_{T} subtraction [Catani, Grazzini (2007)]

$$\delta\sigma^{\mathrm{NNLO}} = \underbrace{\underbrace{\int_{m+2} d\sigma^{RR}}_{\text{double-real}} + \underbrace{\int_{m+1} d\sigma^{RV}}_{\text{real–virtual}} + \underbrace{\int_0^1 dz \int_{m+1} d\sigma^{RC}}_{\text{real–collinear}}}_{\substack{\text{for } q_{\mathrm{T}} \neq 0 \text{ calculable via NLO subtraction,} \\ \text{but divergent for } q_{\mathrm{T}} \to 0}} + \underbrace{\int_m d\sigma^{VV}}_{\text{double-virtual}} + \underbrace{\int_0^1 dz \int_m d\sigma^{VC}}_{\text{virtual–collinear}} + \underbrace{\int_0^1 dz_1 \int_0^1 dz_2 \int_m d\sigma^{CC}}_{\text{double-collinear}}$$

➥ $\sigma^{\mathrm{NLO}}_{F+jet}$

$$= \underbrace{\sigma^{\mathrm{NLO}}_{F+jet}\Big|_{q_{\mathrm{T}}/q\, >\, \mathrm{cut}_{q_{\mathrm{T}}/q}}}_{\substack{\text{integrated exactly using local} \\ \text{NLO subtraction scheme}}} + \underbrace{\sigma^{\mathrm{NLO}}_{F+jet}\Big|_{q_{\mathrm{T}}/q\, \leq\, \mathrm{cut}_{q_{\mathrm{T}}/q}}}_{\substack{\text{approximated by results known} \\ \text{from } q_{\mathrm{T}} \text{ resummation}}} + \underbrace{\int_m d\sigma^{VV} + \int_0^1 dz \int_m d\sigma^{VC} + \int_0^1 dz_1 \int_0^1 dz_2 \int_m d\sigma^{CC}}_{\substack{\text{identified with corresponding terms} \\ \text{in } q_{\mathrm{T}} \text{ resummation}}}$$

NNLO QCD cross section via q_T subtraction

Schematic formula for the NNLO cross section via q_T subtraction [Catani, Grazzini (2007)]

$$\delta\sigma^{\mathrm{NNLO}} \approx \underbrace{\underbrace{\int_{m+2} d\sigma^{RRA}\Big|_{q_T/q\,>\,\mathrm{cut}_{q_T/q}}}_{\Rightarrow\ \delta\sigma^{\mathrm{RRA}}} + \underbrace{\int_{m+1} d\sigma^{RVA}\Big|_{q_T/q\,>\,\mathrm{cut}_{q_T/q}}}_{\Rightarrow\ \delta\sigma^{\mathrm{RVA}}} + \underbrace{\int_0^1 dz \int_{m+1} d\sigma^{RCA}\Big|_{q_T/q\,>\,\mathrm{cut}_{q_T/q}}}_{\Rightarrow\ \delta\sigma^{\mathrm{RCA}}}}_{\text{finite NLO contribution (F+jet), explicit } \mathrm{cut}_{q_T/q} \text{ dependence} \ \Rightarrow\ \delta\sigma^{\mathrm{NLO}}_{F+jet}}$$

$$+ \underbrace{\int_0^1 dz_1 \int_0^1 dz_2 \int_m \left(\frac{\alpha_S}{\pi}\right)^2 \int_{\mathrm{cut}_{q_T/q}}^{\infty} d(q_T/q)\, \boldsymbol{\Sigma}^{(2)}(q_T/q) \otimes d\sigma_{\mathrm{LO}}}_{\text{assigned to Born phase-space, contains up to 1-loop amplitudes, implicit } \mathrm{cut}_{q_T/q} \text{ dependence} \ \Rightarrow\ \delta\sigma^{\mathrm{CT2}}} + \underbrace{\int_0^1 dz_1 \int_0^1 dz_2 \int_m \left(\frac{\alpha_S}{\pi}\right)^2 \mathcal{H}_F^{(2)} \otimes d\sigma_{\mathrm{LO}}}_{\text{contains (finite) 2-loop part, no } \mathrm{cut}_{q_T/q} \text{ dependence} \ \Rightarrow\ \delta\sigma^{\mathrm{VT2}}}$$

- **Local (dipole) subtraction** cancels infrared divergences on the real-emission phase space **(F+jet)**
- **Non-local q_T subtraction** mediates remaining **infrared divergences** between phase spaces through a **slicing cut on q_T/q** ➥ cancellation happens only on the integrated level

Numerical challenges in NNLO slicing – strategy in Munich/Matrix

Numerical implementation of q_T slicing in Matrix

- cross sections/distributions calculated at fixed $\mathrm{cut}_{q_T/q}$ values suffer from power corrections
  - smaller $\mathrm{cut}_{q_T/q}$ values provide more accurate predictions
  - smaller $\mathrm{cut}_{q_T/q}$ values make numerical integration more challenging

➥ compromise between smaller power corrections (prefers lower $\mathrm{cut}_{q_T/q}$) and more stable numerical integration (prefers higher $\mathrm{cut}_{q_T/q}$) required

➥ strategy (both for inclusive cross sections and distributions):

1. simultaneously scan over a range of $\mathrm{cut}_{q_T/q}$ values
2. perform a fit to achieve the result for $\mathrm{cut}_{q_T/q} \to 0$ through an extrapolation

Remarks

- lowest $\mathrm{cut}_{q_T/q}$ value determines performance of integration for contributions with explicit $\mathrm{cut}_{q_T/q}$ dependence
- predictions for power corrections can improve the performance of the method
  - larger minimal $\mathrm{cut}_{q_T/q}$ values can be sufficient
  - extrapolation procedure already mildens effect of power corrections

  ➥ useful, but not essential for processes investigated so far at NNLO

Numerical challenges in NNLO slicing – VT2 contribution

VT2 $$\int_0^1 dz_1 \int_0^1 dz_2 \int_m \left(\frac{\alpha_S}{\pi}\right)^2 \mathcal{H}_F^{(2)} \otimes d\sigma_{\mathrm{LO}}$$

- most challenging ingredient: numerically stable two-loop amplitudes

➥ talk by Vasily Sotnikov

  - ideally with checks of stability and a sophisticated rescue system
    ➥ re-evaluation with higher computational precision if required, e.g. VVAMP [Gehrmann, von Manteuffel, Tancredi (2015)]
  - interpolation grids very efficient: basically zero runtime at integration stage
    ➥ difficult beyond $2 \to 2$ processes due to multi-dimensional interpolation
- some contributions, in particular in context of associated heavy-quark pair production, not known analytically
  ➥ numerical on-the-fly integration, e.g. SHARK [Devoto, Mazzitelli (to appear)] for soft function
- other contributions often with larger numerical impact, but much lower runtimes
  ➥ separate evaluation can significantly reduce overall runtime
- VT2 contribution has no $\mathrm{cut}_{q_\mathrm{T}/q}$ dependence
  ➥ even for most complicated processes not the contribution that dominates overall runtime ...
  ➥ availability of two-loop amplitudes decouples from checks for numerical feasibility

Numerical challenges in NNLO slicing – CT2 contribution

CT2 $$\int_0^1 dz_1 \int_0^1 dz_2 \int_m \left(\frac{\alpha_S}{\pi}\right)^2 \int_{\mathrm{cut}_{q_\mathrm{T}/q}}^{\infty} d(q_\mathrm{T}/q)\, \boldsymbol{\Sigma}^{(2)}(\boldsymbol{q}_\mathrm{T}/\boldsymbol{q}) \otimes d\sigma_{\mathrm{LO}}$$

- assigned to Born phase space, no recoil included (source of fiducial power corrections)
  - ➥ integration over q_T/q can be performed independently of the phase space integration
  - ➥ simultaneous results for all desired $\mathrm{cut}_{q_\mathrm{T}/q}$ values with almost no effort
- involves only tree and 1-loop amplitude for the partonic Born processes
  (also loop×Born 2-colour correlators, Born×Born 3- and 4-colour correlators, etc. for heavy-quark processes)
  - ➥ not the highest complexity of 1-loop amplitudes, no extreme phase space regions
  - ➥ still not irrelevant in terms of runtime, at least for more involved processes
- dependence on $\mathrm{cut}_{q_\mathrm{T}/q}$ implicit, but affects required precision for this counterterm contribution
  - ➥ numerical cancellation against real-emission contributions only on integrated level
- separate evaluation of parts of this contribution can significantly reduce overall runtime
  - ➥ for complicated processes, 1-loop amplitudes time-consuming, but not necessarily numerically dominant

Numerical challenges in NNLO slicing – RCA contribution

RCA $$\int_0^1 dz \int_{m+1} d\sigma^{RCA}\Big|_{q_\mathrm{T}/q\,>\,\mathrm{cut}_{q_\mathrm{T}/q}}$$

- standard $K + P$ terms from dipole subtraction, for the real-emission contribution (F+jet)
- explicit $\mathrm{cut}_{q_\mathrm{T}/q}$ dependence, i.e. numerical implementation through a phase space cut on q_T/q
- integrations over collinear emissions to be arranged such that only one real phase space point is involved
- large contribution for low $\mathrm{cut}_{q_\mathrm{T}/q}$ values due to integration quite close to a phase space singularity
  - ➥ complexity of amplitudes only tree level, thus not really challenging

Numerical challenges in NNLO slicing – RVA contribution

RVA $$\int_{m+1} d\sigma^{RVA}\Big|_{q_\mathrm{T}/q\,>\,\mathrm{cut}_{q_\mathrm{T}/q}}$$

- finite (through adding standard I-operator) virtual contribution, for the real-emission contribution (F+jet)
- explicit $\mathrm{cut}_{q_\mathrm{T}/q}$ dependence, i.e. numerical implementation through a phase space cut on q_T/q
- large contribution for low $\mathrm{cut}_{q_\mathrm{T}/q}$ values due to integration quite close to a phase space singularity
  - ➥ potentially challenging since stable 1-loop amplitudes are required in these limits
    - OpenLoops2 [Buccioni, Lang, Lindert, Maierhöfer, Pozzorini, Zhang, Zoller (2019)] so far sufficient for all applications
      - ➥ on-the-fly tensor reduction [Buccioni, Pozzorini, Zoller (2018)] with hybrid-precision stability system
    - Recola2 with tensor reduction from Collier (not particularly optimized for beyond-NLO applications) performs also reasonably well (not tested excessively)
- RVA contribution typically requires second-most runtime

Numerical challenges in NNLO slicing – RRA contribution

RRA $$\int_{m+2} d\sigma^{RRA}\Big|_{q_{\mathrm{T}}/q\,>\,\mathrm{cut}_{q_{\mathrm{T}}/q}}$$

- real correction for the real-emission contribution (F+jet), finite through standard dipole subtraction terms
  - ➥ different kinematics for each dipole term, coincide with original phase space point only in respective limits
- explicit $\mathrm{cut}_{q_{\mathrm{T}}/q}$ dependence, i.e. numerical implementation through a phase space cut on q_{T}/q
  - ➥ $\mathrm{cut}_{q_{\mathrm{T}}/q}$ acts individually on each dipole, i.e. miscancellations happen even for inclusive cross sections
- only tree-level amplitudes involved, but local cancellation between real and dipole contributions
  - ➥ technical cut on invariants related to singular configurations, $s_{ij}/\hat{s} > \sim 10^{-12}$
- efficient phase space integration over RRA contribution dominates the achievable overall precision
  - ➥ need to deal with peaked integrand structure due to phase space cuts (in particular $\mathrm{cut}_{q_{\mathrm{T}}/q}$)
    - multi-channel approach with topologies based both on real and dipole kinematics
    - additional importance sampling on most of the integration variables
    - further refinements required for involved multi-leg processes
      - pre-optimization of a-priori weights according to resonance structure
      - protection mechanism against over-optimization of channel weights
      - phase space generation (and – if required – weight evaluation) in quad precision

Performance features of the MUNICH phase space integrator

Issue of poorly populated regions

- sample case: high-energy tails
- standard phase space optimization samples points in bulk region

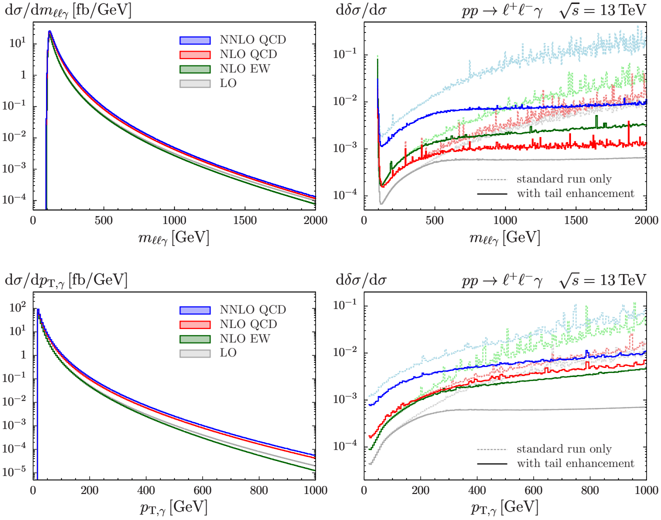
Solution in MUNICH integrator

- additional runs with optimization including a general bias factor
- sophisticated automated combination with results from standard runs

Significantly improved errors

- $\mathcal{O}(10)$ and better with doubled runtime
- simultaneous enhancement of observables

Good performance also for off-shell regions of intermediate resonances



Numerical challenges in NNLO slicing – extrapolation procedure

Remarks on extrapolation procedure applied in MATRIX

- Goal: remove the dependence on power corrections for fixed $\mathrm{cut}_{q_\mathrm{T}/q}$ values, which limit the accuracy
  ➥ in principle removed by extrapolation $\mathrm{cut}_{q_\mathrm{T}/q} \to 0$, but replaced by an extrapolation uncertainty
- free parameters in extrapolation procedure
  - functional form of fitting curve
    ➥ compromise between expected behaviour and predictivity of fit under real-life conditions
  - lowest $\mathrm{cut}_{q_\mathrm{T}/q}$ value used in fit
    ➥ minimal possible value fixed by runs, but allowing the lowest values to be ignored can be useful
  - highest $\mathrm{cut}_{q_\mathrm{T}/q}$ value used in fit chosen in a given range through least χ^2/dof
    ➥ variation of largest included $\mathrm{cut}_{q_\mathrm{T}/q}$ value used for estimate of extrapolation error
- error estimate based on range variation and individual integration errors at fixed $\mathrm{cut}_{q_\mathrm{T}/q}$ values
  ➥ also extrapolation range and gradient at lowest $\mathrm{cut}_{q_\mathrm{T}/q}$ value taken into account
  ➥ chosen to provide reliable estimates also for low-statistics runs
- typical number of $\mathrm{cut}_{q_\mathrm{T}/q}$ values calculated in MATRIX: $\mathcal{O}(100)$ for inclusive cross sections, $\mathcal{O}(10)$ for differential distributions ➥ limitation from memory and disk space

Investigation of $r_{\mathrm{cut}} = \mathrm{cut}_{q_T/q}$ dependence — sample case $\mathrm{pp} \to \gamma\gamma + X$

Result for $r_{\mathrm{cut}} \to 0$ via extrapolation

- automated and simultaneous scan over reasonable range of r_{cut} values
- quadratic least-χ^2 fit with variable range

$$\sigma_{\mathrm{(N)NLO}}(r_{\mathrm{cut}}) = A r_{\mathrm{cut}}^2 + B r_{\mathrm{cut}} + \sigma_{\mathrm{(N)NLO}}$$

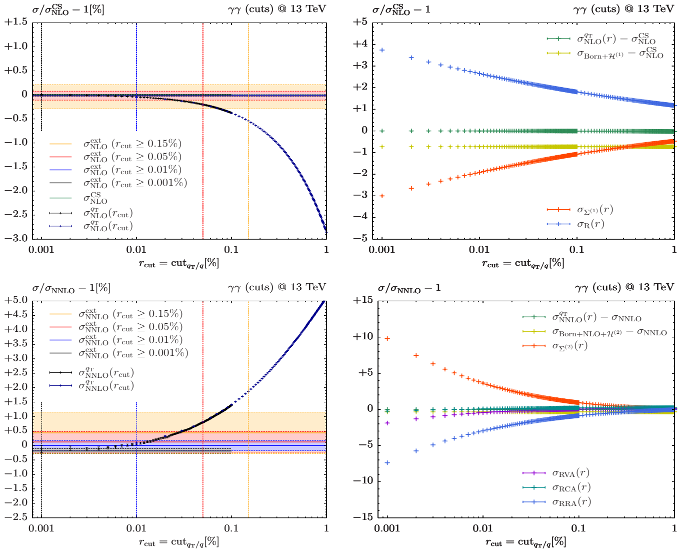
- error estimate based on combination of statistical error and variation of r_{cut} range

➥ **Significant r_{cut} dependence for processes involving isolated photons**

➥ talk by Gherardo Vita

➥ good agreement of extrapolated results within errors for different start values

- $r_{\mathrm{cut}} \geq 0.15\%$
- $r_{\mathrm{cut}} \geq 0.05\%$
- $r_{\mathrm{cut}} \geq 0.01\%$
- $r_{\mathrm{cut}} \geq 0.001\%$



Investigation of $r_{\mathrm{cut}} = \mathrm{cut}_{q_T/q}$ dependence — sample case $\mathrm{pp} \to \ell^-\ell^+\ell'^-\ell'^+ + X$

Result for $r_{\mathrm{cut}} \to 0$ via extrapolation

- same procedure for all processes

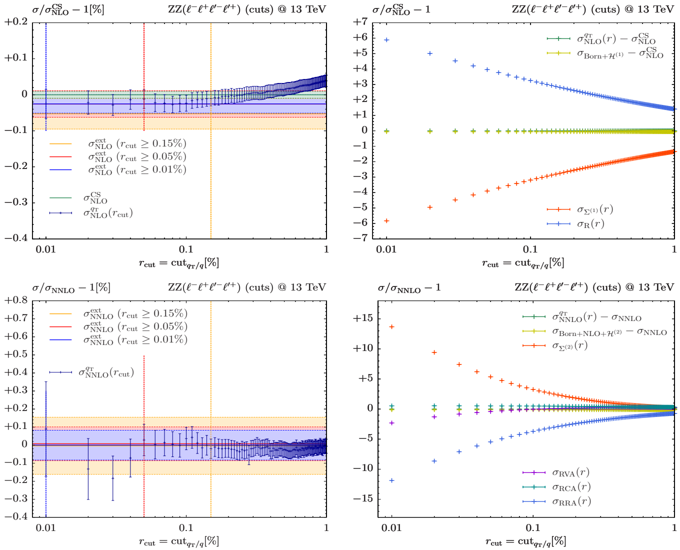
$$\sigma_{\mathrm{(N)NLO}}(r_{\mathrm{cut}}) = A r_{\mathrm{cut}}^2 + B r_{\mathrm{cut}} + \sigma_{\mathrm{(N)NLO}}$$

➥ **No significant r_{cut} dependence for processes without isolated photons**

➥ good agreement of extrapolated results within errors for different start values

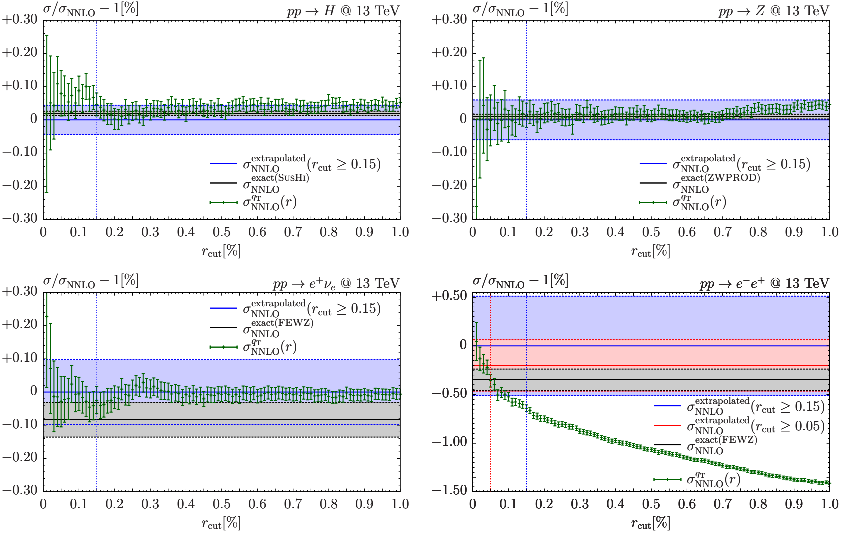
- $r_{\mathrm{cut}} \geq 0.15\%$
- $r_{\mathrm{cut}} \geq 0.05\%$
- $r_{\mathrm{cut}} \geq 0.01\%$

- larger cancellation between contributions (factor of ≈ 15 at $r_{\mathrm{cut}} = 0.01\%$)
- **Important exception:** linear power corrections induced by particular fiducial cut configurations



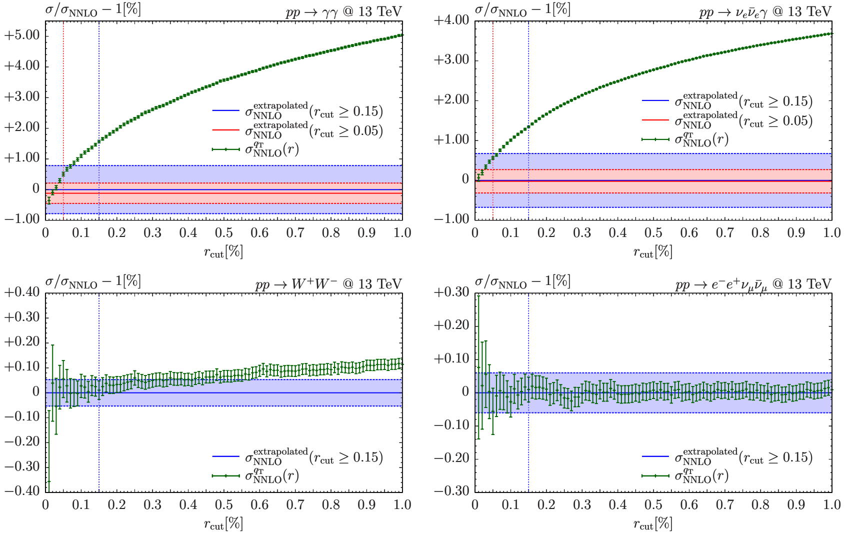
Automatic $r_{\text{cut}} \to 0$ extrapolation in MATRIX – H/V production

- **Simple quadratic fit** $(A \times r_{\text{cut}}^2 + B \times r_{\text{cut}} + C)$ applied for $r_{\text{cut}} \to 0$ extrapolation
- **Error estimate** based on statistical error and variation of uppermost r_{cut} value
- Vertical dotted lines (blue, red) indicate lowest r_{cut} used in extrapolation
- Slicing-independent reference results (black)



Automatic $r_{\rm cut} \to 0$ extrapolation in MATRIX – VV production

- **Simple quadratic fit** $(A \times r_{\rm cut}^2 + B \times r_{\rm cut} + C)$ applied for $r_{\rm cut} \to 0$ extrapolation
- **Error estimate** based on statistical error and variation of uppermost $r_{\rm cut}$ value
- Vertical dotted lines (blue, red) indicate lowest $r_{\rm cut}$ used in extrapolation

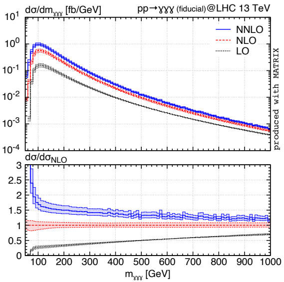


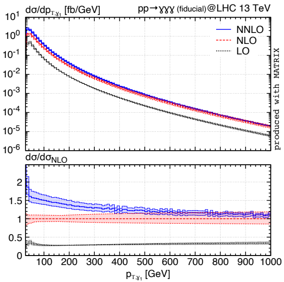
Triphoton production at NNLO QCD accuracy

First calculation for genuine 2 → 3 process at NNLO QCD with q_T subtraction in MATRIX

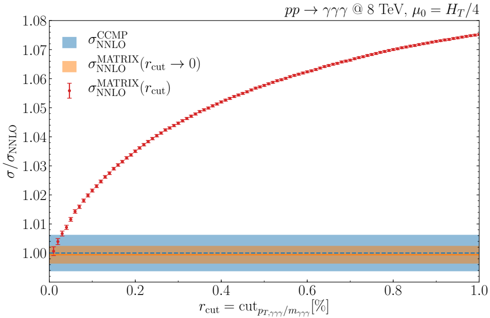
- fast and stable 2-loop amplitudes [Abreu, Page, Pascual, Sotnikov (2021)] generated with CARAVEL, using PENTAGONFUNCTIONS++
  [Abreu et al. (2020)] [Chicherin, Sotnikov (2020)]
- good numerical control over slicing parameter dependence
- full agreement with independent calculation (also validated on the level of differential distributions)
  [Chawdhry, Czakon, Mitov, Poncelet (2020)]

[SK, Sotnikov, Wiesemann (2021)]





[SK, Sotnikov, Wiesemann (2021)]



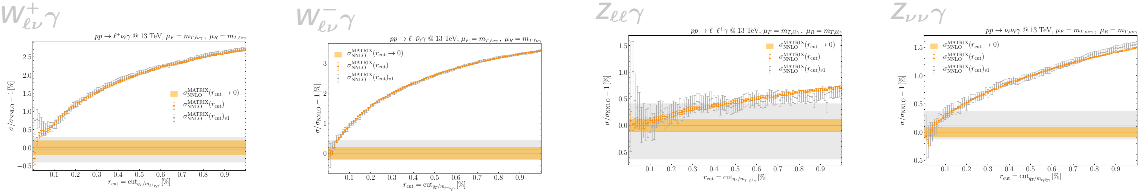
- great numerical performance also with fine resolution and in suppressed phase space regions (tail enhancement feature applied)

➥ **MATRIX fully suitable for triboson processes**

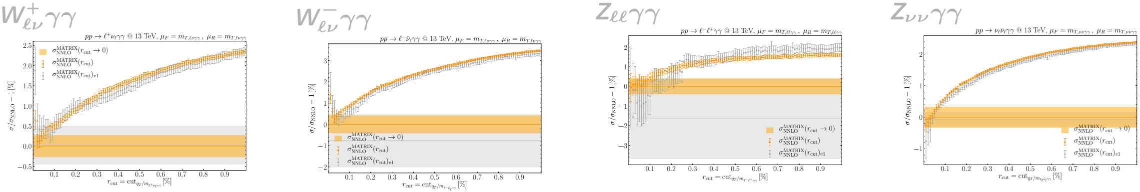
Feasibility studies on $V\gamma\gamma$ production processes at NNLO QCD accuracy

Studies on r_{cut} dependence for $V\gamma\gamma$ processes (standard cuts and photon isolation)

- diboson processes ($V\gamma$): impact of finite remainder of two-loop amplitudes small, only $\mathcal{O}(2-3\%)$



- triboson processes ($V\gamma\gamma$): finite remainder of two-loop amplitudes set to zero

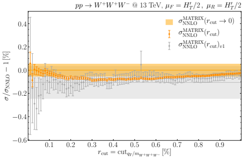


➥ comparable precision for NNLO QCD predictions achievable for $V\gamma\gamma$ processes as for $V\gamma$

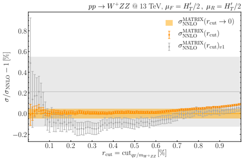
Feasibility studies on massive triboson production at NNLO QCD accuracy

Studies on $r_{\rm cut}$ dependence for inclusive massive VVV production processes

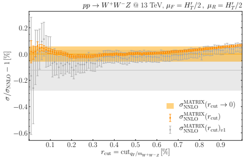
$W^+W^+W^-$



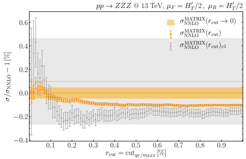
W^+ZZ



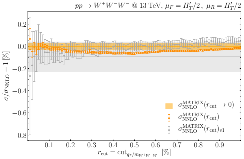
W^+W^-Z



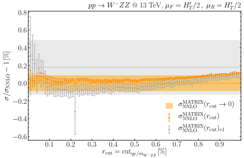
ZZZ



$W^+W^-W^-$



W^-ZZ



finite remainder of two-loop amplitudes set to zero for these technical feasibility studies
(typically small, only $\mathcal{O}(2\%)$ for VV processes)

➥ obviously, no robust conclusion on the size of NNLO QCD corrections can be drawn without knowledge of the two-loop amplitudes

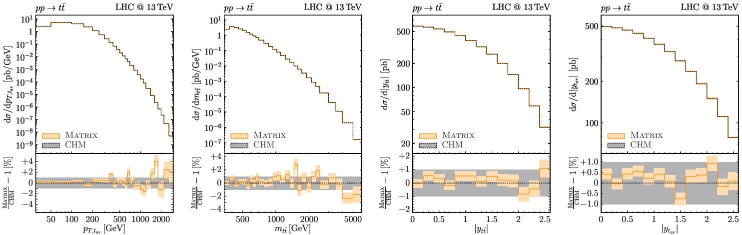
- very good numerical control ➥ permille-level precision achievable within reasonable runtimes
- results with significantly lower statistics are shown in gray to illustrate that extrapolation procedure is quite stable against fluctuations ➥ good agreement within assigned error bands

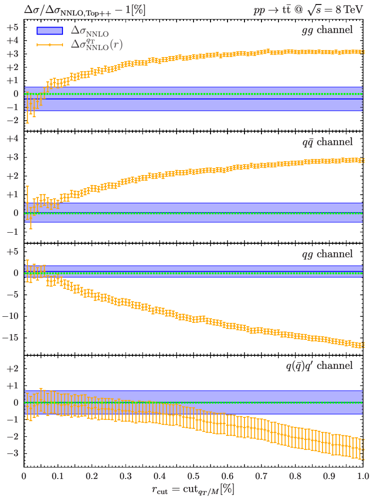
Top-quark pair production at NNLO QCD accuracy

First MATRIX calculation for colourful final states at NNLO QCD

[Catani, Devoto, Grazzini, SK, Mazzitelli, Sargsyan (2019)]

- 2-loop amplitudes from numerical result [Bärnreuther, Czakon, Fiedler (2014)]
- slicing parameter dependence under good numerical control; investigation after splitting into partonic channels
  - ➥ full agreement with TOP++ [Czakon, Mitov (2014)]
- successful validation also on the level of differential distributions [Catani, Devoto, Grazzini, SK, Mazzitelli (2019)]
  (comparison against results from [Czakon, Heymes, Mitov (2017)])

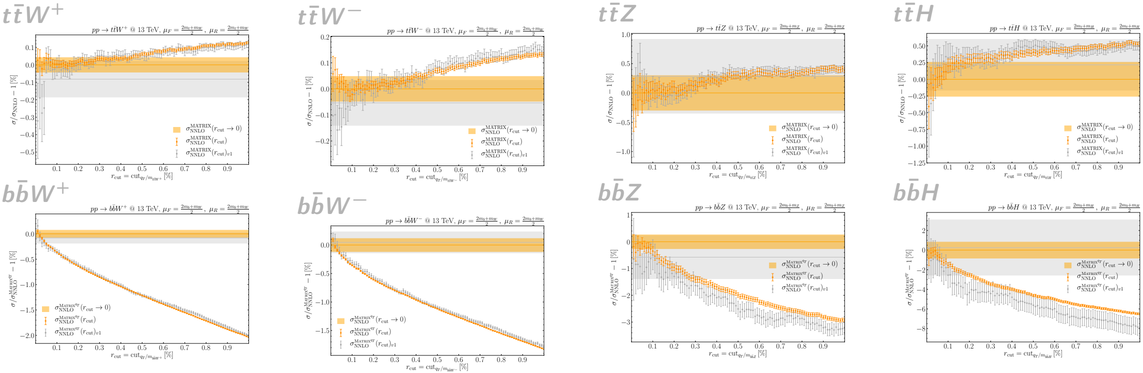




Feasibility studies on associated heavy-quark pair production at NNLO QCD accuracy

Studies on r_{cut} dependence for inclusive $Q\bar{Q} + X$ processes

- proof-of-principle for non-diagonal channels in $t\bar{t}H$ [Catani, Fabre, SK, Grazzini (2021)]



- finite remainders of two-loop amplitudes and of the soft function neglected in these studies
  - ➥ no reliable estimate of NNLO QCD result, just to illustrate numerical control over $r_{\mathrm{cut}} \to 0$ extrapolation
    - ➥ precision well below a percent achievable within reasonable runtimes

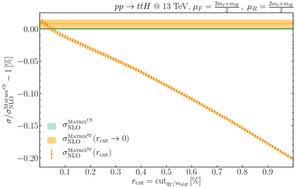
$t\bar{t}H$ production at NNLO QCD accuracy

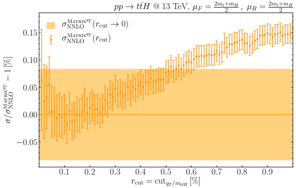
First MATRIX calculation for $Q\bar{Q}X$ at NNLO QCD

- exact calculation, apart from finite remainder of the two-loop amplitude treated in a soft-boson approximation
  [Catani, Devoto, Grazzini, SK, Mazzitelli, Savoini (2022)]

  ➥ talk by C. Savoini

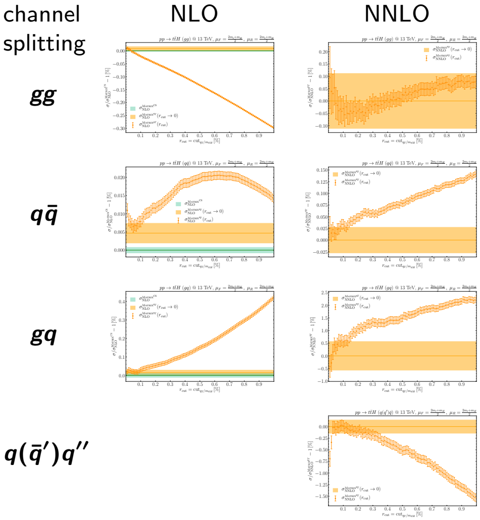
  ➥ SA error estimate of $\lesssim 1\%$ wrt. NNLO cross section





- good numerical control of NNLO cross section: $\mathcal{O}(0.1\%)$

  ➥ some peculiarities in individual channels (also at NLO), but overall impact extremely small ...



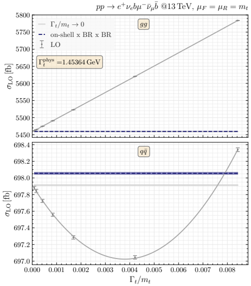
Studies towards off-shell $t\bar{t}$ production at NNLO QCD accuracy – NLO validation

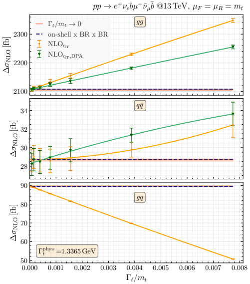
$W^+W^-b\bar{b}$ at NNLO QCD belongs to $Q\bar{Q}X$ process class ➥ in principle feasible in MATRIX

[Buonocore, Devoto, Grazzini, SK, Lindert, Mazzitelli, Savoini (preliminary)]

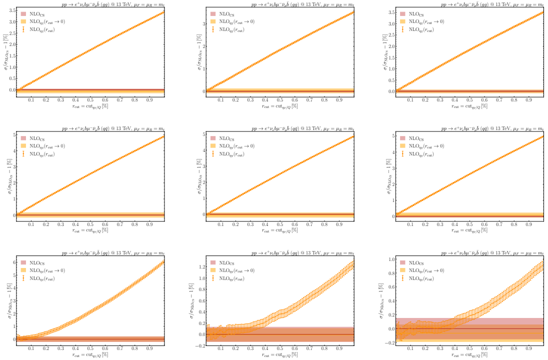
- 2-loop amplitudes out of reach
  - ➥ double-pole approximation (DPA)
- numerically challenging $2 \to 4$ process with intermediate top resonances

➥ validation at NLO against on-shell (NWA) $t\bar{t}$ result through $\Gamma_t \to 0$ extrapolation





$\Gamma_t / \Gamma_{t,\mathrm{phys}}$	1	0.1	0.01
gg			
$q\bar{q}$			
gq			



➥ good numerical control over $r_{\rm cut} \to 0$ at NLO

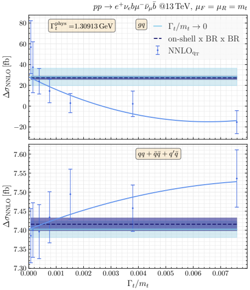
➥ reasonable agreement with NWA in $\Gamma_t \to 0$ limit

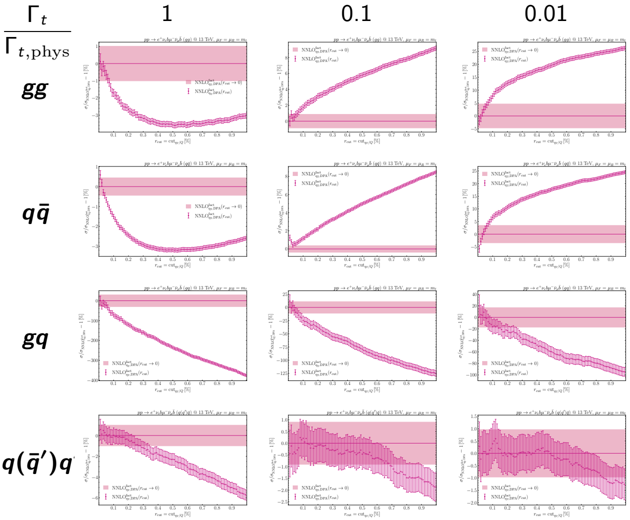
Studies towards off-shell $t\bar{t}$ production at NNLO QCD accuracy – NNLO validation

[Buonocore, Devoto, Grazzini, SK, Lindert, Mazzitelli, Savoini (in progress)]

Towards $W^+W^-b\bar{b}$ at NNLO QCD

- DPA implementation at NNLO incomplete
- calculation of non-diagonal channels exact
  - ➥ validation against on-shell (NWA) $t\bar{t}$ result through $\Gamma_t \to 0$ extrapolation





- ➥ good agreement with NWA in $\Gamma_t \to 0$ limit
- ➥ reasonable numerical control over $r_{\text{cut}} \to 0$

Recoil-driven linear power corrections in neutral-current Drell–Yan process

Transverse-momentum cuts on undistinguished particles in two-body final states introduce enhanced sensitivity to low momentum scales [Salam, Slade (2021)]

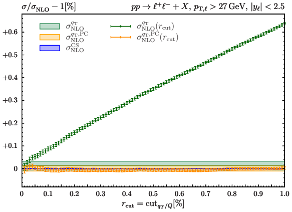
- **Linear power corrections (linPCs) in context of q_T subtraction**
  - have been resummed to all orders for s-channel (DY, Higgs) production [Ebert, Michel, Stewart, Tackmann (2021); Billis, Dehnadi, Ebert, Michel, Tackmann (2021)]
- **Recoil prescription** can be used to predict linPCs also in fixed-order calculations [Buonocore, SK, Rottoli, Wiesemann (2022), Camarda, Cieri, Ferrera ('21)] :

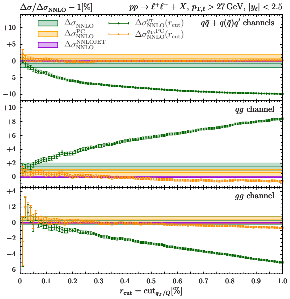
$$\Delta\sigma^{\text{linPCs}}(r_{\text{cut}}) = \int d\Phi_F \int_{\epsilon}^{r_{\text{cut}}} dr' \left(\frac{d\sigma^{\text{CT}}}{d\Phi_F\, dr'}\, \Theta_{\text{cuts}}(\Phi_F^{\text{rec}}) - \frac{d\sigma^{\text{CT}}}{d\Phi_F\, dr'}\, \Theta_{\text{cuts}}(\Phi_F) \right)$$

  - Φ_F^{rec} describes frame where system F is assigned a recoil q_T (boost from Collins–Soper frame, but precise prescription irrelevant)

- **Adding the contribution $\Delta\sigma^{\text{linPCs}}(r_{\text{cut}})$ reduces leading (recoil-driven) r_{cut} dependence from linear (without linPCs) to (at most) quadratic**
  - Illustration for **symmetric cuts** at NLO (upper plot) and NNLO (lower plot; reference result from NNLOjet [Bizon et al. (2021)])

[Buonocore, SK, Rottoli, Wiesemann (2022)]





Distributions with linPCs for neutral-current DY process with symmetric cuts

Sample distribution: ℓ^+ rapidity at NLO (left) and NNLO (right)

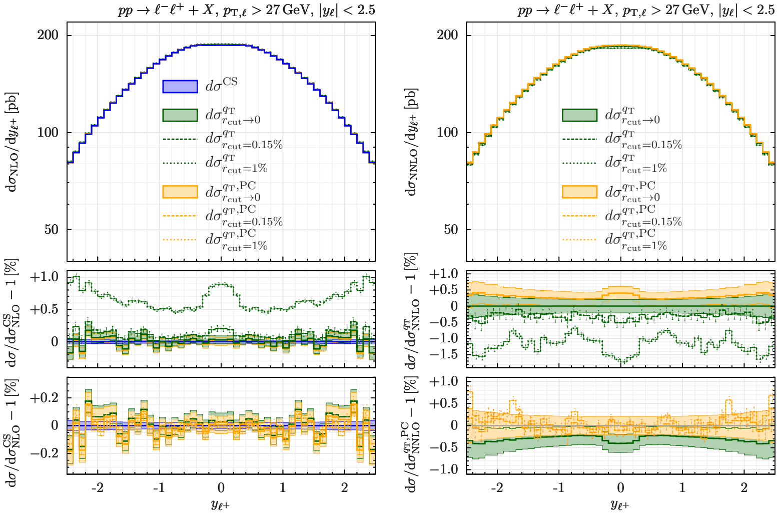
- up to $\sim 2\%$ deviations for highest considered value $r_{\text{cut}} = 1\%$ without linPCs
- good agreement between considered r_{cut} values with linPCs (within errors)

Note: The extrapolated results with linPCs and without linPCs agree well within errors!

➡ **higher efficiency with linPCs (larger r_{cut} values sufficient)**

➡ **accurate results also from binwise extrapolation without including linPCs**

[Buonocore, SK, Rottoli, Wiesemann (2022)]

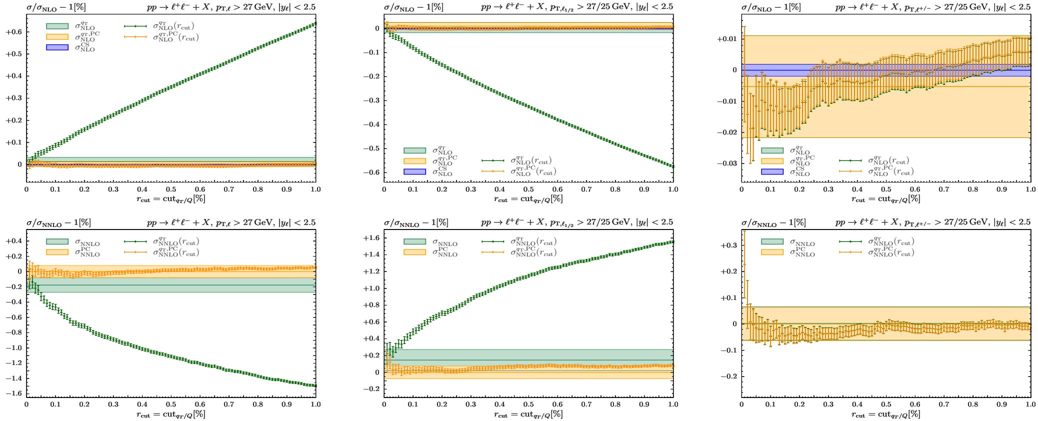


Recoil-driven linear power corrections for different fiducial cut configurations

symmetric ($p_{T,\ell} > 27$ GeV) **asymmetric** ($p_{T,\ell_{1/2}} > 27/25$ GeV) **staggered** ($p_{T,\ell^\pm} > 27/25$ GeV)

NLO

NNLO



[Buonocore, SK, Rottoli, Wiesemann (2022)]

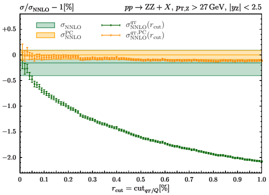
- similarly sizable linPCs (with opposite sign) for **symmetric** and **asymmetric** cuts
- **linPCs absent for staggered cuts** (as long as $q_T < \delta p_T$) ➥ also for other alternative cuts [Salam, Slade (2021)]

Recoil-driven linear power corrections for diboson processes

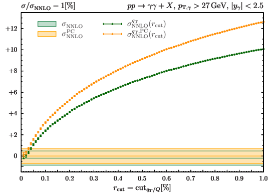
Investigation of linPCs for diboson processes

(two-body kinematics and symmetric cuts)

ZZ



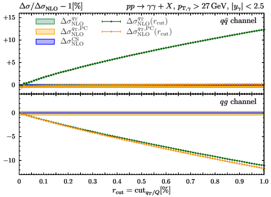
γγ



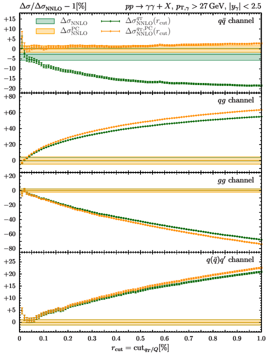
- For ZZ production, linPCs from recoil prescription reduce $r_{\rm cut}$ dependence to (at most) quadratic
  - ➥ formally proven only for s-channel production [Ebert, Michel, Stewart, Tackmann (2021)]
- For $\gamma\gamma$ production, $r_{\rm cut}$ dependence from photon isolation dominates over recoil-driven linPCs

Breakdown into partonic channels for $\gamma\gamma$ case

[Buonocore, SK, Rottoli, Wiesemann (2022)]



↑ NLO NNLO →



➥ linear $r_{\rm cut}$ dependence in $q\bar{q}$ channel only due to kinematic effects

➥ cured by recoil-driven linPCs for $q\bar{q}$ channel

Note: Recoil-driven linPCs absent for staggered cuts (e.g. on $|y|$-ordered bosons), like in Drell–Yan case

Conclusions & Outlook

Numerical challenges in NNLO (q_T) slicing

- stable 2-loop amplitudes (no slicing-cut dependence, i.e. clearly not slicing approach dependent)
- stable 1-loop amplitudes, in particular close to divergent phase space regions ➡ very small $cut_{q_T/q}$ values
- stable phase space integration of the subtracted double-real contribution
  ➡ only tree-level amplitudes, but different subtraction term phase spaces with very small $cut_{q_T/q}$ values

➡ **numerical control over $F+\mathrm{jet}$ calculation at NLO crucial for feasibility of NNLO calculations**

Sample applications and feasibility studies for NNLO calculations

- single-boson, diboson, triboson production
- (associated) heavy-quark pair production

➡ **$2 \to 3$ processes (and possibly even beyond) feasible within reasonable runtimes**

Inclusion of power corrections in NNLO (q_T) slicing

- can improve performance, since higher $cut_{q_T/q}$ values might provide sufficient accuracy

➡ **not so crucial (but still useful) at NNLO, but presumably very important beyond NNLO**

Backup

Backup

The MUNICH/MATRIX framework for automated NNLO calculations

MATRIX — MUNICH Automates qT-subtraction and Resummation to Integrate X-sections
[Grazzini, SK, Wiesemann (2018)]

- public tool to perform fully differential NNLO QCD calculations for a large class of processes
- core of the framework: the C++ parton-level Monte Carlo generator
  MUNICH — MUlti-chaNnel Integrator at swiss (CH) precision [SK]
  - bookkeeping of partonic subprocesses for all contributions
  - fully automated dipole subtraction for NLO calculations (massive, QCD and EW)
    [Catani, Seymour (1997), Catani, Dittmaier, Seymour, Trocsanyi (2002), Dittmaier (2000), SK, Lindert, Maierhöfer, Pozzorini, Schönherr (2015)]
  - general amplitude interface 1-loop amplitudes 2-loop amplitudes
  - highly efficient multi-channel Monte Carlo integration with several optimization features
  - simultaneous monitoring of slicing parameter and automated extrapolation
- PYTHON script to simplify the use of MATRIX
  - installation of MUNICH and all supplementary software
  - interactive shell steering all run phases without human intervention (grid-, pre-, main-run, summary)
  - organization of parallelized running on multicore machines and commonly used clusters:
    SLURM, HTCONDOR, LSF, etc.

Supplying MUNICH/MATRIX with 1-loop amplitudes

Process-independent interfaces to general automated amplitude generators

- OPENLOOPS [Cascioli, Maierhöfer, Pozzorini (2012); SK, Lindert, Maierhöfer, Pozzorini, Schönherr (2015)] v2 [Buccioni, Lang, Lindert, Maierhöfer, Pozzorini, Zhang, Zoller (2019)], written in FORTRAN
  - general code and process libraries
  - on-the-fly tensor reduction [Buccioni, Pozzorini, Zoller (2018)] with hybrid-precision stability system
  - scalar integrals from COLLIER [Denner, Dittmaier, Hofer (2006); Denner, Dittmaier (2011)] or ONELOOP [van Hameren (2011)]
- RECOLA [Actis, Denner, Hofer, Lang, Scharf, Uccirati (2017)] v2 [Denner, Lang, Uccirati (2017)], written in FORTRAN
  - on-the-fly generation of amplitudes
  - tensor reduction and scalar integrals via COLLIER [Denner, Dittmaier, Hofer (2006); Denner, Dittmaier (2003, 2006, 2011)]
  - different model files available, also for SMEFT and BSM applications
- modular structure of MUNICH allows other generators to be interfaced as well

Several dedicated interfaces developed in context of MATRIX applications

- loop$\times$tree and loop$\times$loop colour (and spin) correlators
- helicity amplitudes, colour-stripped amplitudes to construct 4-colour correlators
- imaginary parts of loop$\times$tree amplitudes and correlators, helicity-flip amplitudes

Interfacing dedicated 2-loop amplitudes to MUNICH/MATRIX

- Higgs, Drell–Yan, **VH**, $\gamma\gamma$, **V**γ production
  - direct implementation of public analytic results, e.g. for Vγ [Gehrmann, Tandredi (2012)]
- **VV** production — qqVVAMP [Gehrmann, von Manteuffel, Tancredi (2015)] and ggVVAMP [von Manteuffel, Tancredi (2015)] libraries
  - C++ libraries using GINAC [Bauer, Frink, Kreckel (2002); Vollinga, Weinzierl (2005)] and CLN for arbitrary precision arithmetics
  - IBP approach, generated using MATHEMATICA, FORM [Vermaseren et al.], REDUZE2 [von Manteuffel, Studerus ('12)]
  - independent calculation of amplitudes in [Caola, Henn, Melnikov, Smirnov, Smirnov (2015; 2016)]
  - Higgs-mediated helicity amplitudes with full m_t dependence from [Harlander, Prausa, Usovitsch (2019; 2020)]
- $\gamma\gamma\gamma$ production — amplitudes from [Abreu, Page, Pascual, Sotnikov ('20)]
  - C++ library, generated by CARAVEL [Abreu et al. (2020)], applying PENTAGONFUNCTIONS++ [Chicherin, Sotnikov (2020)]
  - numerical unitarity and analytic reconstruction techniques [Ita (2015); Abreu et al. (2018; 2018; 2019; 2019)]
- **HH** production (full m_t dependence) — HHGRID library [Borowka, Greiner, Heinrich, Jones, Kerner, Schlenk, Schubert, Zirke (2016)]
  - PYTHON based numerical interpolation of amplitude grid
  - generated by 2-loop extension of GOSAM [Jones (2016)], REDUZE2 [von Manteuffel, Studerus ('12)], SECDEC3 [Borowka et al. (2015)]
- $\mathbf{Q\bar{Q}}$ production — amplitude grids from [Bärnreuther, Czakon, Fiedler (2014)]
  - FORTRAN routine for numerical interpolation of 2-dimensional grid, improved by expansions