A critical appraisal of NLO+PS matching

Particle Physics Seminar, Zürich

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Based on

arXiv:1111.1220 (Stefan Höche, Frank Krauss, Marek Schönherr, FS)

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Motivation for NLO+PS matching

Two approaches to higher-order corrections

Fixed order ME calculation

+ Exact to fixed order

- + Includes all interferences
- + $N_C = 3$ (summed or sampled)
- + Includes virtual contributions
- Perturbation breaks down in logarithmically enhanced regions
- Only low FS multiplicity

Parton Shower

- + Resums logarithmically enhanced contributions to all orders
- + High-multiplicity final state
- + Allows for exclusive hadron-level events
- Only approximation for emission ME
- Large N_C limit
 - ₩

Goal: Combine advantages

- Include virtual contributions and hard QCD radiation from NLO ME
- Keep intrajet evolution provided by the PS

Fixed order calculations (NLO)

Reminder + Notation: Subtraction method

- ► Contributions to NLO cross section: Born, Virtual and Real emission
- V and R divergent in separate phase space integrations ⇒ Subtraction method for expectation value of observable O at NLO:

$$\begin{split} \langle O \rangle^{(\mathrm{NLO})} &= \sum_{\tilde{f_B}} \int \mathrm{d}\Phi_B \left[\mathcal{B}(\Phi_B) + \tilde{\mathcal{V}}(\Phi_B) + \sum_{\tilde{ij}} \mathcal{I}_{\tilde{ij}}^{(\mathrm{S})}(\Phi_B) \right] O(\Phi_B) \\ &+ \sum_{\tilde{f_R}} \int \mathrm{d}\Phi_R \left[\mathcal{R}(\Phi_R) O(\Phi_R) - \sum_{\{ij\}} \mathcal{D}_{ij}^{(\mathrm{S})}(\Phi_R) O(b_{ij}(\Phi_R)) \right] \end{split}$$

- ► Subtraction terms D and their integrated form I given e.g. by Frixione-Kunszt-Signer or Catani-Seymour
- Subtraction defines phase space mappings $\Phi_R \stackrel{b_{ij}}{\underset{r_{ij}}{\longrightarrow}} \left(\Phi_B, \Phi_{R|B}^{ij} \right)$

Resummation in parton-showers

Factorisation of collinear QCD emissions

Universal factorisation of QCD real emission ME in collinear limit:

$$\mathcal{R} \stackrel{ij \text{ collinear}}{\longrightarrow} \mathcal{D}_{ij}^{(\mathrm{PS})} = \mathcal{B} \times \left(\sum_{\{ij\}} \frac{1}{2p_i p_j} 8\pi \alpha_s \, \mathcal{K}_{ij}(p_i, p_j) \right)$$

- ▶ Sum over subterms *ij* of the factorisation, e.g. parton lines (DGLAP)
- $\frac{1}{2p_i p_j}$ from massless propagator Evolution variable of shower $t \sim 2p_i p_j$ (e.g. k_{\perp} , angle, ...)
- K_{ij} splitting kernel for branching ij → i + j Specific form depends on scheme of the factorisation, e.g.:
 - Altarelli-Parisi splitting functions
 - Dipole terms from Catani-Seymour subtraction (in $N_C \rightarrow \infty$)
 - Antenna functions

Radiative phase space factorisation:

$$\mathrm{d}\Phi_R \to \mathrm{d}\Phi_B \ \mathrm{d}\Phi_{R|B}^{ij} \stackrel{\mathrm{e.g.}}{=} \mathrm{d}\Phi_B \ \frac{1}{16\pi^2} \ \mathrm{d}t \ \mathrm{d}z \frac{\mathrm{d}\phi}{2\pi}$$

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Resummation in parton-showers

Differential branching probability

$$\mathrm{d}\sigma_{\mathrm{branch}}^{\tilde{\imath}j} = \sum_{f_i = q,g} \mathrm{d}\Phi_{R|B}^{ij} \; \frac{\mathcal{D}_{ij}^{(\mathrm{PS})}}{\mathcal{B}}$$

Symmetry factors/PDFs ignored)

Differential probability for single branching of subterm ij in interval $d\Phi_{R|B}^{ij}$

Total "survival" probability of parton ensemble

- Integrate single branching probability down to scale t in terms of $t(\Phi_{R|B}^{ij})$
- ► Assume multiple independent emissions (Poisson statistics) ⇒ Exponentiation

subterm:
$$\begin{split} \Delta_{ij}^{(\mathrm{PS})}(t) &= 1 - \int \mathrm{d}\sigma_{\mathrm{branch}}^{\tilde{\imath}j} \,\Theta\left(t(\Phi_{R|B}^{ij}) - t\right) + \dots \\ &= \exp\left\{-\sum_{f_i=q,g} \int \mathrm{d}\Phi_{R|B}^{ij} \,\Theta\left(t(\Phi_{R|B}^{ij}) - t\right) \,\frac{\mathcal{D}_{ij}^{(\mathrm{PS})}}{\mathcal{B}}\right\} \\ \text{event:} \quad \Delta^{(\mathrm{PS})}(t) \,= \,\prod_{ij} \Delta_{ij}^{(\mathrm{PS})}(t) \end{split}$$

Resummation in parton-showers

Cross section up to first emission in a parton shower

$$\left\langle O\right\rangle^{(\mathrm{PS})} = \int \mathrm{d}\Phi_B \, \mathcal{B}\left[\underbrace{\Delta(t_0) \, O(\Phi_B)}_{\mathrm{unresolved}} + \underbrace{\sum_{\tilde{ij}} \sum_{f_i} \int_{t_0}^{\mu_F^2} \mathrm{d}\Phi_{R|B}^{ij} \, \frac{\mathcal{D}_{ij}^{(\mathrm{PS})}}{\mathcal{B}} \Delta(t) \, O\left(r_{\tilde{ij}}(\Phi_B)\right)}_{\mathrm{resolved}}\right]$$

Generating events for $\langle O \rangle^{(\mathrm{PS})}$	Features of $\langle O \rangle^{(\mathrm{PS})}$		
 Generate Born ME event B at μ_F² Generate t according to survival probability Δ(t)/Δ(μ_F²) Stop if t < t₀ Generate remaining kinematics of the branching (z, φ) according to D^(PS)_{ij}/B 	 Unitarity: [] _{D=1} = 1 ⇒ LO cross section preserved "Unresolved" part: No emissions above cutoff t₀ "Resolved" part: Emission between t₀ and µ_F² in PS approximation 		

From fixed order to resummation

Problem

► Applying PS resummation to *B* event was simple (for some definition of simple)

• At NLO, can the same simply be done separately for $\mathcal{B}, \mathcal{V} + \mathcal{I}, \mathcal{R} - \mathcal{D}$?

$$\begin{split} \langle O \rangle^{(\text{NLO})} &= \sum_{\tilde{f_B}} \int \mathrm{d}\Phi_B \left[\mathcal{B}(\Phi_B) + \tilde{\mathcal{V}}(\Phi_B) + \sum_{\tilde{ij}} \mathcal{I}_{\tilde{ij}}^{(\text{S})}(\Phi_B) \right] O(\Phi_B) \\ &+ \sum_{\tilde{f_R}} \int \mathrm{d}\Phi_R \left[\mathcal{R}(\Phi_R) O(\Phi_R) - \sum_{\{ij\}} \mathcal{D}_{ij}^{(\text{S})}(\Phi_R) O(b_{ij}(\Phi_R)) \right] \end{split}$$

 Different observable dependence in *R* and *D* but if showered separately \Rightarrow "double counting"

Solution: Let's in the following ...

- rewrite $\langle O \rangle^{(\text{NLO})}$ a bit
- ▶ add some PS resummation into the game leading to $\langle O \rangle^{(\text{NLO}+\text{PS})}$ and claim that:
 - $\langle O \rangle^{(\text{NLO}+\text{PS})} = \langle O \rangle^{(\text{NLO})}$ to $\mathcal{O}(\alpha_s)$
 - $\langle O \rangle^{(\text{NLO}+\text{PS})}$ contains the first step of a PS evolution which can then be continued trivially with a regular PS
- sketch how $\langle O \rangle^{(\text{NLO}+\text{PS})}$ is being generated in MC@NLO and POWHEG ►

Results Conclusions

From fixed order to resummation

First rewrite: Additional set of subtraction terms $\mathcal{D}^{(A)}$

$$O^{(\text{NLO})} = \sum_{\vec{f}_B} \int d\Phi_B \, \bar{\mathcal{B}}^{(\text{A})}(\Phi_B) \, O(\Phi_B) \\ + \sum_{\vec{f}_R} \int d\Phi_R \left[\mathcal{R}(\Phi_R) \, O(\Phi_R) - \sum_{\{ij\}} \mathcal{D}_{ij}^{(\text{A})}(\Phi_R) \, O\left(b_{ij}(\Phi_R)\right) \right]$$

with $\bar{\mathcal{B}}^{(A)}(\Phi_B)$ defined as:

$$\begin{split} \bar{\mathfrak{Z}}^{(\mathsf{A})}(\Phi_B) &= \mathcal{B}(\Phi_B) + \tilde{\mathcal{V}}(\Phi_B) + \sum_{\{ij\}} \mathcal{I}^{(\mathsf{S})}_{ij}(\Phi_B) \\ &+ \sum_{\{ij\}} \sum_{f_i = q, g} \int \mathrm{d}\Phi^{ij}_{R|B} \left[\mathcal{D}^{(\mathsf{A})}_{ij}(r_{ij}(\Phi_B)) - \mathcal{D}^{(\mathsf{S})}_{ij}(r_{ij}(\Phi_B)) \right] \end{split}$$

▶ D^(A)_{ij} must have same kinematics mapping as D^(S)_{ij}

- Exact choice of $\mathcal{D}_{ij}^{(A)}$ will later specify MC@NLO vs. POWHEG
- ▶ Issue with different observable kinematics not yet solved \rightarrow next step

Results Conclusions

From fixed order to resummation

Second rewrite: Make observable correction term explicit

$$\langle O \rangle^{(\text{NLO})} = \sum_{\vec{f}_B} \int d\Phi_B \, \vec{\mathcal{B}}^{(\text{A})}(\Phi_B) \, O(\Phi_B)$$

$$+ \sum_{\vec{f}_R} \int d\Phi_R \left[\mathcal{R}(\Phi_R) - \sum_{\{ij\}} \mathcal{D}_{ij}^{(\text{A})}(\Phi_R) \right] \, O(\Phi_R)$$

$$+ \langle O \rangle^{(\text{corr})}$$

with $\langle O \rangle^{(\text{corr})}$ defined as:

$$\langle O \rangle^{(\text{corr})} = \sum_{\vec{f}_R} \int \mathrm{d}\Phi_R \sum_{\{ij\}} \mathcal{D}_{ij}^{(\mathrm{A})}(\Phi_R) \left[O(\Phi_R) - O(b_{ij}(\Phi_R)) \right]$$

- Explicit correction term due to observable kinematics: $\langle O \rangle^{(\text{corr})}$
- Essence of NLO+PS
 - Ignore $\langle O \rangle^{(\text{corr})}$ for the time being
 - Apply PS resummation to first line using $\Delta^{(A)}$ in which $\mathcal{D}^{(PS)} \to \mathcal{D}^{(A)}$

Results Conclusion:

From fixed order to resummation

Master formula for NLO+PS up to first emission

$$\begin{split} \langle O \rangle^{(\mathrm{NLO}+\mathrm{PS})} &= \sum_{\vec{f}B} \int \mathrm{d}\Phi_B \, \vec{\mathcal{B}}^{(\mathrm{A})}(\Phi_B) \left[\underbrace{\Delta^{(\mathrm{A})}(t_0)}_{\mathrm{unresolved}} O(\Phi_B) \\ &+ \sum_{\{\vec{i}j\}} \sum_{f_i} \int_{t_0} \mathrm{d}\Phi^{ij}_{R|B} \underbrace{\frac{\mathcal{D}^{(\mathrm{A})}_{ij}(r_{\vec{i}j}(\Phi_B))}{\mathcal{B}(\Phi_B)} \, \Delta^{(\mathrm{A})}(t)}_{\mathrm{resolved, singular}} O(r_{\vec{i}j}(\Phi_B)) \right] \\ &+ \sum_{\vec{f}R} \int \mathrm{d}\Phi_R \underbrace{\left[\mathcal{R}(\Phi_R) - \sum_{ij} \mathcal{D}^{(\mathrm{A})}_{ij}(\Phi_R) \right]}_{\mathrm{resolved, singular}} O(\Phi_R) \end{split}$$

resolved, non-singular

- This is generated in the following way:
 - ▶ Generate seed event according to first or second line of ⟨O⟩^(NLO) on last slide
 - Second line: \mathbb{H} -event with Φ_R is kept as-is \rightarrow resolved, non-singular term
 - First line: S-event with Φ_B is processed through one-step PS with Δ^(A) ⇒ emission (resolved, singular) or no emission (unresolved) above t₀
- To $\mathcal{O}(\alpha_s)$ this reproduces $\langle O \rangle^{(\text{NLO})}$ including the correction term
- Resolved cases: Subsequent emissions can be generated by ordinary PS

Special case: MC@NLO

Choice of $\mathcal{D}^{(A)}$

Choose the additional subtraction terms as

$$\mathcal{D}_{ij}^{(\mathrm{A})} \to \mathcal{D}_{ij}^{(\mathrm{S})}$$

Comments

- $\bar{\mathcal{B}}^{(A)}$ simplified significantly
- Still non-trivial to implement, need either of:
 - One-step PS algorithm based on subtraction terms D^(S)_{ij}
 ! splitting kernels can become negative ⇒ ∆ > 1 !
 - ME subtraction using ordinary PS kernels D^(PS)_{ij}
 soft divergences (subleading in ¹/_{NC}) not covered !
- In SHERPA's MC@NLO implementation:
 - D^(S) from Catani-Seymour
 - Weighted $N_C = 3$ one-step PS to generate $\Delta > 1$

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Special case: POWHEG

Original POWHEG

Choose additional subtraction terms as

$$\mathcal{D}_{ij}^{(A)}(\Phi_R) \to \rho_{ij}(\Phi_R) \mathcal{R}(\Phi_R) \quad \text{where} \quad \rho_{ij}(\Phi_R) = \frac{\mathcal{D}_{ij}^{(S)}(\Phi_R)}{\sum_{mn} \mathcal{D}_{mn}^{(S)}(\Phi_R)}$$

- Ill-term vanishes
- ▶ B^(A) remains complicated now, includes real-emission integration (may be done by Monte-Carlo method)
- Similar to PS with ME-correction for 1st emission (e.g. Herwig, Pythia)

Mixed scheme

 \blacktriangleright Subtract arbitrary regular piece from ${\cal R}$ and generate separately

$$\mathcal{D}_{ij}^{(A)}(\Phi_R) \to \rho_{ij}(\Phi_R) \ [\mathcal{R}(\Phi_R) - \mathcal{R}^r(\Phi_R)] \qquad \text{where} \qquad \rho_{ij} \text{ as above}$$

- ▶ Allows to generate the non-singular cases of \mathcal{R} without underlying \mathcal{B}
- More control over how much is exponentiated

Subtleties to note

Exponentiation uncertainty

- Have to exponentiate full subtraction terms D^(S)_{ij} (MC@NLO) or even R (POWHEG) for NLO accuracy
- Exponent contains arbitrary terms beyond all-orders singular pieces = Systematic theory uncertainty in NLO+PS
- \Rightarrow Studied in detail in Results later

Renormalisation scale choice in NLO vs. PS

- First emission partly done by NLO matrix element, partly by PS
- $\alpha_s^{(\text{NLO})}(\mu_R)$ taken at fixed scale
- α_s^(PS)(k_⊥) taken at transverse momentum of the branching (partially resums soft higher-order contributions)
- \Rightarrow Only noted here without solution, critical for smooth NLO \otimes NLO merging

NLO+PS uncertainties

Perturbative uncertainties

- Unknown higher-order corrections
- Estimated here by simultaneous scale variations $\mu_F = \mu_R = \frac{1}{2}\mu \dots 2\mu$

 $\rightsquigarrow pp \rightarrow h$ + jet later

Non-perturbative uncertainties

- Model uncertainties in hadronisation, hadron decays, multiple parton interactions
- Estimated here by variation of parameters/models within tuned ranges

 $\rightsquigarrow pp \rightarrow W$ + jet later

Exponentiation uncertainties

- Arbitrariness of D^(A) and thus of the exponent in Δ^(A)
- Estimated here using SHERPA by:
 - Comparing MC@NLO and POWHEG
 - Using MC@NLO with variable "dipole α_{cut} " restriction in $\mathcal{D}^{(S)}$: $\alpha_{cut} \rightarrow 0$ decreases phase space for non-singular contributions

	Results	
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Exponentiation uncertainties in the example of $gg \rightarrow h$

Example setup

- $\blacktriangleright ~gg \rightarrow h \rightarrow \tau \tau$ at LHC with $\sqrt{s}=7$ TeV and $m_h=120$ GeV, $\mu=m_h$
- Analysed with $p_{\perp}^{\tau}>25~{\rm GeV}$ and $|n^{\tau}|<3.5$
- ▶ Jets defined using inclusive k_{\perp} with R = 0.7 and $p_{\perp} > 20$ GeV

Studies at parton shower level

- 1. Validate NLO+PS against fixed NLO predictions
- 2. Comparison with LO parton shower (LO+PS)
- 3. MC@NLO vs. POWHEG
- 4. MC@NLO with $0.001 \le \alpha_{\text{cut}} \le 1$ variation

```
\Rightarrow Very busy plots
(SORRY!)
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Results Conclusions

Exponentiation uncertainties in the example of $gg \rightarrow h$



- Surprising result: Huge NLO+PS uncertainties especially at large p^h_⊥
- POWHEG and unrestricted MC@NLO similar
- $\blacktriangleright\,$ Decreasing exponentiation of non-singular pieces with $\alpha_{\rm cut} \lesssim 0.01$ recovers NLO behaviour
- Resummation region p^h_⊥ → 0 strongly affected by α_{cut} variation: side effect of imperfect functional form of α (vs. parton shower t ~ k²_⊥)

Results Conclusion

Exponentiation uncertainties in the example of $gg \rightarrow h$



▶ Predictions separated by H and S events for illustration purposes

		Results	
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Exponentiation uncertainties in the example of $gg \rightarrow h$



- Predictions much more stable for y_h than for p^h_⊥
- Observable already exists at LO, thus described at NLO here

Exponentiation uncertainties in the example of $gg \rightarrow h$



- Large uncertainties for $\Delta y(h, j)$
- Interesting dip structure in MC@NLO due to cuts on exponentiated phase space Surprisingly similar to effect from dead zones in MC@NLO with HERWIG

Predictions for $pp \rightarrow h$ + jet

Example setup

- ▶ $pp \rightarrow h[\rightarrow \tau \tau]$ + jet at LHC with $\sqrt{s} = 7$ TeV and $m_h = 120$ GeV, $\mu = p_{\perp}^{j_{\text{lead}}}$
- Virtual matrix element interfaced from MCFM
- Generated ME level with $p_{\perp} > 10$ GeV for inclusive k_{\perp} jets with R = 0.5
- Analysed with p[↑]_⊥ > 25 GeV and |n[↑]| < 3.5, jets defined using inclusive k_⊥ with R = 0.7 and p_⊥ > 20 GeV

Studies

- $\blacktriangleright\,$ Includes hadronisation, hadron decays, multiple parton interactions (MPI), QED corrections to $h\to\tau\tau\,$ decay
- Scale uncertainty band (yellow) from $\mu_F = \mu_R = \frac{1}{2}\mu \dots 2\mu$
- Exponentiation uncertainty band (gray) from $\alpha_{cut} = 0.001 \dots 1$

Results Conclusio

Predictions for $pp \rightarrow h + \text{jet}$



- Despite NLO accuracy, large exponentiation uncertainty for large p_{\perp} :
 - ► Large influence from higher-order corrections in △ where more phase space is exponentiated
 - Additional distortion from scale difference for real-emission: relative p_⊥ of partons vs. p_⊥ against beam

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Results Conclusion

Predictions for $pp \rightarrow h + \text{jet}$



- Milder exponentiation variations in $\Delta \eta$ (h, jet), mainly normalisation due to larger emission rates with $\alpha_{cut} \rightarrow 1$
- $\Delta \phi$ (jet 1, jet 2): Back-to-back situation amplified due to harder radiation

Non-perturbative effects in W + jet production

Example setup

- $pp \rightarrow W[\rightarrow e\nu]$ + jet at LHC with $\sqrt{s} = 7$ TeV, $\mu = p_{\perp}^{j_{\text{lead}}}$
- Virtual matrix element interfaced from BlackHat
- Exponentiation level fixed at α_{cut} = 0.03
- Generated ME level with $p_{\perp} > 10$ GeV for inclusive k_{\perp} jets with R = 0.5
- Analysed jets with $p_{\perp} > 20$ GeV for inclusive k_{\perp} jets with R = 0.7

Non-perturbative effects

"Parton Level"	Only seed event + first emission off S-events in MC@NLO
"Shower Level"	PL + all QCD emissions in the parton shower and QED emissions in the YFS approach
"Shower+MPI"	SL + multiple parton interactions and intrinsic p_{\perp} of the beam hadron
"Hadron Level"	Additionally, hadronisation and hadron decays are included

Results Conclu

Non-perturbative effects in W + jet production



Properties of the W-boson virtually unaffected

Results Conclust

Non-perturbative effects in W + jet production



- Jet properties changed significantly by non-perturbative effects
- Hadronisation and MPI partially compensate each other, depends on jet algorithm
- \Rightarrow How large is the uncertainty?

Results Concl

Hadronisation uncertainties in W + jet production



- Probe hadronisation uncertainties by switching from SHERPA default cluster fragmentation to Lund string
- Differences negligible for all jet observables studied, except the specifically sensitive jet mass

Results Conclus

Comparison to data for W + jet production



- Comparison to ATLAS data (arXiv:1012.5382): Good agreement in shape, discrepancies in jet rates
- ► Especially two/three jet rates too low: Only predicted at LO/PS
- ► MPI parameter variations plotted as yellow band ⇒ negligible

Comparison to data for Z + jet production

Example setup

- $pp \rightarrow Z$ + jet at Tevatron with $\sqrt{s} = 1.96$ TeV, $\mu = p_{\perp}^{j_{\text{lead}}}$
- Virtual matrix element interfaced from BlackHat
- Exponentiation level fixed at $\alpha_{cut} = 0.03$
- Generated ME level with p⊥ > 10 GeV for inclusive k⊥ jets with R = 0.5

Tevatron analyses

- CDF Z+jets arXiv:0711.3717
- ▶ DØ Z+jet arXiv:0808.1296
- DØ Z+jets arXiv:0903.1748
- ▶ DØ Z+jet arXiv:0907.4286

Results Conclusion

Comparison to data for Z + jet production



- Z-boson properties in Z+jet+X production
- ▶ Fair agreement, 10% rate deficiency
- MPI uncertainties largest at low $p_{\perp}(Z)$

Results Conclus

Comparison to data for Z + jet production



- One-jet-rate too low by 10-20%
- ▶ Not conclusive on shape of leading jet p⊥
- Reminder: Large exponentiation uncertainties

Results Co

Comparison to data for Z + jet production



- Angular correlations of Z-boson and leading jet
- Shape of rapidity distributions matched fairly well
- Significant deviations for azimuthal correlation: Back-to-back works, but $\Delta \phi < \pi$ is underestimated. That region is generated by emissions beyond the first one \Rightarrow only LO/PS accuracy

Conclusions

Summary

- NLO+PS matching was presented in common formalism
- POWHEG and MC@NLO developed as special cases
- Uncertainties from exponentiation ambiguities are large but understood
- Scale and non-perturbative uncertainties relatively small
- ► First NLO+PS predictions for *h* + jet
- ► W/Z + jet compared to experimental data

Outlook

- Improved functional form of dipole α could allow for better limitation of exponentation
- ► Merging NLO+PS with higher-multiplicity tree-level MEs can provide better description of multi-jet final states (→ e.g. MENLOPS)
- Ultimate goal: Merging of NLO at different multiplicities + parton shower