

RECENT PROGRESS IN HIGHER-ORDER CALCULATIONS*

* impossible to cover everything; personal selection

Workshop on Tools for High Precision LHC Simulations — October 31st 2022

Alexander Huss









SCATTERING REACTIONS O LHC



short distance "hard"

high scales: $10^2 - 10^3$ GeV

evolution towards a physical observable state

- long distance "soft"
- low scales: $\mathcal{O}(\text{few GeV})$

Monte Carlo & Matching, Parton Shower Sessions

non perturbative M. Ubiali, P. Nason

quarks & gluons $\leftrightarrow \rightarrow$ hadrons





SCATTERING REACTIONS O LHC



• **Focus:** high momentum transfer & clean signatures

operturbation theory:

 $\sigma = \sigma_0 \times \left(1 + \alpha_x + \alpha_x^2 + \alpha_x^3 + \dots\right)$ fixed order: LO NLO NNLO N³LO ...

• $\alpha_{\rm s} \sim 0.1 ~\&~ \alpha_{\rm ew} \sim 0.01$

• 1% target $\leftrightarrow \mathcal{O}(\alpha_s^2, \alpha_{ew})$ $\rightarrow \mathcal{O}(\alpha_{\rm s}^3, \alpha_{\rm s}^2, \alpha_{\rm ew})$





THE MASTER FORMULA – COLLINEAR FACTORIZATION



$$\sigma_{AB} = \sum_{ab} \int_0^1 \mathrm{d}x_a \int_0^1 \mathrm{d}x_b f_{a|A}(x_a) f_{b|B}(x_b) \hat{\sigma}_{ab}(x_a, x_b) \left(1 + \mathcal{O}(\Lambda_{\mathrm{QCD}}/Q)\right)$$

parton distribution functions
(non-perturbative, universal)
in principle, improvable

hard scattering (perturbation theory) systematically improvable

$$\hat{f}$$

$$\hat{\sigma}_{ab} = \hat{\sigma}_{ab}^{(0)} + \left(\frac{\alpha_{s}}{2\pi}\right)\hat{\sigma}_{ab}^{(1)} + \left(\frac{\alpha_{s}}{2\pi}\right)^{2}\hat{\sigma}_{ab}^{(2)} + \cdots$$

$$\hat{\sigma}_{ab}$$

$$x_{b}P_{B}$$

$$f_{b|B}(x_{b})$$

$$P_{B}$$

non-perturbative effects (power suppressed) ultimately, limiting factor?



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NLO – CONCEPTUALLY SOLVED?

one-loop amplitudes

(all master integrals known, well understood: log, Li2)





"virtual"



automated 1-loop providers

- Gosam [Chiesa et al. '14]
- MadGraph5_aMC@NLO [Frixione et al. '18]
- NLOX [Honeywell et al. '18]
- OpenLoops [Pozzorini et al. '19]
- Recola [Actis et al. '16]

IR subtraction (involved IR structure, numerical stability, construction)









NLO – PUSHING THE LIMIT*

- off-shell ---> high-multiplicity
 - \hookrightarrow large non-resonance effects?...
 - \hookrightarrow particularly challenging for EW
- $2 \rightarrow 6$ processes
 - ► $pp \rightarrow e^+ \nu_e \mu^- \bar{\nu}_\mu b\bar{b}$ (t \bar{t}) [Denner, Pellen '16]
 - $pp \rightarrow 4\ell jj \text{ (VBS)}$ [Denner et al. '16-22]
 - $pp \to \ell_1^- \bar{\nu}_{\ell_1} \ell_2^+ \nu_{\ell_2} \ell_2^+ \nu_{\ell_3}$ (WWW) [Schönherr '18; Dittmaier et al. '19]
 - $pp \rightarrow e^+e^-\mu^+\nu_\mu jj_b$ (tZj) [Denner, Pelliccioli, Schwan '22]
- $2 \rightarrow 7$ processes
 - $pp \rightarrow e^+ \nu_e \mu^- \bar{\nu}_\mu b\bar{b} H$ (t $\bar{t}H$) [Denner, Lang, Pellen, Uccirati '16]
- $2 \rightarrow 8$ processes
 - $pp \rightarrow e^+ \nu_e \tau^+ \nu_\tau \mu^- \bar{\nu}_\mu b\bar{b} \ (t\bar{t}W)$ [Denner, Pelliccioli '21]

G. Pellicioli * another frontier: loop-induced, polarization, ...







J. Lindert



NNLO – THE BUILDING BLOCKS & CHALLENGES





WHAT CAN WE DO TODAY? — THE NNLO TIMELINE

Tremendous progress in the past $\sim 5-10$ years! \hookrightarrow 2 \rightarrow 2 under good control; 2 \rightarrow 3 good progress



[timeline adapted from M. Grazzini]

K. Ellis (colour-less), D. Lombardi (VV), A. Ratti (bb), J. Mazzitelli (tt), M. Grazzini (ttH), L. Buonocore (massive f.s.), L. Rottoli (f.s. jet)







DIFFERENT METHODS*

- > Antenna [Gehrmann–De Ridder, Gehrmann, Glover '05]
- CoLorFul [Del Duca, Somogyi, Trocsanyi '05]
- ► qT-subtraction

[Catani, Grazzini '07; MATRIX]

- STRIPPER (sector-improved residues) [Czakon '10]
- nested soft-collinear

[Caola, Melnikov, Röntsch '17]

- N-jettiness [Gaunt, Stahlhofen, Tackmann, Walsh '15] [Boughezal, Focke, Liu, Petriello '15; MCFM]
- Projection-to-Born

[Cacciari, et al. '15]

- Geometric, Local analytical Sectors
 [Herzog '18] [Magnea et al. '18]
- * Subtraction & Slicing

INDEPENDENT CALCULATIONS — $H + jet \times 3!$

residue subtraction

[Caola, Melnikov, Schulze '15]



very complex calculations *we* validation!

- long-standing [~'15] discrepancy in H + jet \hookrightarrow only resolved in ['19]
- benchmark approaches

τ_1 jettiness subtraction

[Boughezal, Focke, Giele, Liu, Petriello '15] [Campbell, Ellis, Seth '19]

antenna subtraction

[Chen, Cruz-Martinez, Gehrmann, Glover, Jaquier '16]







INCLUSIVE JETS – 2 CALCULATIONS!





STRIPPER [Czakon, van Hameren, Mitov, Poncelet '19]

- in very good agreement!
- sub-leading colour negligible!(?)





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HOW GOOD IS LEADING COLOUR?



✓ Inclusive Jets

SLC corrections

- \hookrightarrow up to 20% on δ
- \hookrightarrow largest @ low-*p*

impact on NNL $\hookrightarrow \leq 2\%$ & with

✓ Incl. jets (R = 0. ✓ Dijet d σ /d m_{ii} (R sub-leading colour:SLCleading colour:LCfull colour (LC+SLC):FC

[Chen, Gehrmann, Glover, AH, Mo '22]

$$(R = 0.7)$$

Spositive
So^{NNLO}
PT
AO
hin Δ_{scl}

$$(A) = 0.4)$$

$$X \text{ Dijet 3D } (R = 0.7)$$

large SLC corrections
 $\ominus \ low-p_{T,avg} \iff 30-60\%$
 $\ominus \ med-p_{T,avg} \iff 30-60\%$
 $\ominus \ med-p_{T,avg} \iff -20\%$
LC \rightarrow FC
 $\ominus \ 5\%$ enhancement

$$(R = 0.7)$$



Current Frontier: $2 \rightarrow 3$

 $pp \rightarrow \gamma \gamma \gamma$

[Chawdhry, Czakon, Mitov, Poncelet '19]
[Kallweit, Sotnikov, Wiesemann '20]

• $pp \rightarrow \gamma \gamma + j$ [Chawdhry, Czakon, Mitov, Poncelet '21] (gluon-fusion @ NLO \simeq N3LO) \hookrightarrow [Badger, Gehrmann, Marcoli, Moodie '21]



pp → jjjj
 [Czakon, Mitov, Poncelet '21]
 (gg → ggg; antenna automation)
 ← [Chen, Gehrmann, Glover, Huss, Marcoli '22]

 pp → Wbb
 [Hartanto, Poncelet, Popescu, Zoia '22]

 pp → ttH

[Catani, Devoto, Grazzini, Kallweit, Mazzitelli, Savoini '22]

good convergence @ NNLO except: low- $p_{\rm T}^{\gamma\gamma}$, cos $\phi_{\rm CS}$, ...

 \leftrightarrow loop-induced large δ NLO (100%)







$2 \rightarrow 3$ Results at the Frontier

TRI-JET PRODUCTION [Czakon, Mitov, Poncelet '21]

- *most complex* subtraction for $2 \rightarrow 3$
- non-degenerate Born kinematics
 event shapes, TEEC, azimuth. decorr.

•
$$R_{3/2} = \mathrm{d}\sigma_{3j}/\mathrm{d}\sigma_{2j} \iff \alpha_{\mathrm{s}}$$





BEYOND "STANDARD" CALCULATIONS

- adding flavour
 - Z+b-jet [Gauld, Gehrmann-De Ridder, Glover, AH, Majer '20]
 - W+c-jet [Czakon, Mitov, Pellen, Poncelet '20]
- adding masses
 - $pp \rightarrow WH (H \rightarrow bb)$ [Behring, Bizoń, Caola, Melnikov, Röntsch '20]
 - $pp \rightarrow bb$ [Catani, Devoto, Grazzini, Kallweit, Mazzitelli '21]
- identified particles / fragmentation
 - hadron fragmentation [Catani, Devoto, Grazzini, Kallweit, Mazzitelli '21]
 - isolated photons [Gehrmann, Schürmann '22; + Chen, Glover, Höfer, AH '22]
- beyond approximations
 - non-factorizable corrections
 - Higgs beyond HTL $(m_{\rm f}
 ightarrow \infty)$ [Czakon, Harlander, Klappert, Niggetiedt '20]
- NNLO \bigcirc PS separate session



A. Ratti, J. Mazzitelli L. Buonocore

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VBF [Liu, Melnikov, Penin '19]; [Dreyer, Karlberg, Tancredi '20];
                                                                            C.Y. Wang
single-t [Brønnum-Hansen, Melnikov, Quarroz, Signorile-Signorile, Wang '22]
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B-HADRON IN tt

[Czakon, Generet, Mitov, Poncelet '21,'22]



- $t\bar{t} \leftrightarrow high purity \& statistics$
- B-hadrons measured precisely \hookrightarrow precise m_t extraction?
- $m_t \gg m_b$ • small power corrections
- extract $D_{i \to B}$ from e⁺e⁻ data





ISOLATED PHOTONS γ + jet



maybe ok at NLO; matters at NNLO

MIXED QCD-EW CORRECTIONS FOR DRELL-YAN

$$d\sigma = d\sigma_{LO} \left(1 + \left(\frac{\alpha_s}{2\pi}\right) \delta^{(1,0)} + \left(\frac{\alpha}{2\pi}\right) \delta^{(0,1)} + \left(\frac{\alpha_s}{2\pi}\right)^2 \delta^{(2,0)} + \left(\frac{\alpha_s}{2\pi}\right) \left(\frac{\alpha}{2\pi}\right) \delta^{(1,1)} + \cdots \right)$$

notation

resonant / on-shell

- pole expansion [Dittmaier, Huss, Schwinn '14,'15]
- on-shell Z (OCD×OED) [Delto, Jaquier, Melnikov, Röntsch '19]
- σ_{Z}^{tot} [Bonciani, Buccioni, Rana, Vicini '20]
- on-shell

[Buccioni, Caola, Delto, Jaquier, Melnikov, Roentsch '20] [Behring, Buccioni, Caola, Delto, Jaquier, Melnikov, Röntsch '20]

$$\begin{split} \sigma^{\text{NLO}_{\text{s}\oplus\text{ew}}} &\sim 1, \ \delta^{(1,0)}, \ \delta^{(0,1)} \\ \sigma^{\text{NNLO}_{\text{s}\otimes\text{ew}}} &\sim 1, \ \delta^{(1,0)}, \ \delta^{(0,1)}, \ \delta^{(1,1)} \\ \sigma^{\text{NNLO}_{\text{s}\otimes\text{ew}}}_{\text{naive prod.}} &\sim 1, \ \delta^{(1,0)}, \ \delta^{(0,1)}, \ \delta^{(1,0)} \times \delta^{(0,1)} \end{split}$$

off-shell

W

[Buonocore, Grazzini, Kallweit, Savoini, Tramontano '21]

Ζ

[Bonciani, Buonocore, Grazzini, Kallweit, Rana, Tramontano, Vicini '21] [Buccioni, Caola, Chawdhry, Devoto, Heller, von Manteuffel, Melnikov, Rontsch, Signorile-Signorile '22]

$\mathcal{O}(\alpha_{s} \alpha) - \text{Resonance Region}$

- kinematic effects

[Bonciani, Buonocore, Grazzini, Kallweit, Rana, Tramontano, Vicini '21]

naive product not able to capture

 \hookrightarrow fails below resonance $(m_{\ell\ell})$ \hookrightarrow fails away from shoulder $(p_{\rm T}^{\mu})$

pole approximation (PA) \hookrightarrow well-captures full result here

N³LO – A NEW FRONTIER

$$f \qquad \left(\frac{\alpha_{s}}{2\pi}\right)^{3} \hat{\sigma}_{ab}^{(3)} \iff \text{ largely limited to } "2 \to 1$$

$$\hat{\sigma}_{ab} \times x_{b} P_{B} \qquad B \qquad f_{b|B}(x_{b}) \qquad P_{B}$$

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N3LO INCLUSIVE CROSS SECTIONS

• $gg \rightarrow H \checkmark$

[C. Anastasiou, C. Duhr, F. Dulat, F. Herzog, B. Mistlberger '15] VBF-H ✓, VBF-HH ✓ 100 PDF4LHC15_nnlo_mc $Q/2 < \mu_R$, $\mu_F < 2~Q$ [F. Dreyer, A. Karlberg '16, '18] • $b\bar{b} \rightarrow H \checkmark$ 10 [C. Duhr, F. Dulat, B. Mistlberger '19] • $pp \rightarrow \gamma^*$? $pp \rightarrow W^{\pm}$? LO [C. Duhr, F. Dulat, B. Mistlberger '20] NLO $gg \rightarrow HH \checkmark$ 1.02 atio to N3LO [L. Chen, H. Li, H. Shao, J. Wang '20] 1.01 • pp $\rightarrow \gamma^*/Z$? [C. Duhr, B. Mistlberger '21] 0.99 $pp \rightarrow VH$? 10 13 7 20 [J. Baglio, C. Duhr, B. Mistlberger, R. Szafron '22]

DRELL-YAN @ N3LO - SCALE & PDF DEPENDENCE [Baglio, Duhr, Mistlberger, Szafron '22]

* similar for W⁻

resonance region $\leftrightarrow \rightarrow$ non-overlapping bands; Δ_{i}

180 $Q \; [{
m GeV}]$

$$_{\rm scl}^{\rm NNLO} \simeq \Delta_{\rm scl}^{\rm N^3LO}$$
 ?!

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DRELL-YAN @ N3LO - SCALE & PDF DEPENDENCE [Baglio, Duhr, Mistlberger, Szafron '22]

	Q [GeV]	$\delta\sigma^{ m N^3LO}$	$\delta\sigma^{\rm NNLO}$	$\delta(\text{scale})$	$\delta(\text{PDF} + \alpha_S)$	$\delta(\text{PDF-TH})$
$gg \to \text{Higgs}$	m_H	3.5%	30%	$+0.21\% \\ -2.37\%$	$\pm 3.2\%$	$\pm 1.2\%$
$b\bar{b} \rightarrow \text{Higgs}$	m_H	-2.3%	2.1%	$+3.0\% \\ -4.8\%$	$\pm 8.4\%$	$\pm 2.5\%$
NCDY	30	-4.8%	-0.34%	$+1.53\% \\ -2.54\%$	$+3.7\% \\ -3.8\%$	$\pm 2.8\%$
	100	-2.1%	-2.3%	$+0.66\%\ -0.79\%$	$+1.8\% \\ -1.9\%$	$\pm 2.5\%$
$CCDY(W^+)$	30	-4.7%	-0.1%	$+2.5\% \\ -1.7\%$	$\pm 3.95\%$	$\pm 3.2\%$
	150	-2.0%	-0.1%	$+0.5\%\ -0.5\%$	$\pm 1.9\%$	$\pm 2.1\%$
$\operatorname{CCDY}(W^{-})$	30	-5.0%	-0.1%	$+2.6\% \\ -1.6\%$	$\pm 3.7\%$	$\pm 3.2\%$
	150	-2.1%	-0.6%	$+0.6\%\ -0.5\%$	$\pm 2\%$	$\pm 2.13\%$

- *K*-factors (N³LO/NNLO) ~ $2-5\% \rightarrow \text{important for }\%$ -level target!
- $\Delta_{\rm scl} \sim {\rm few} \%$
- PDF uncertainties ~ 2–9% (+ few % from missing N³LO PDFs)

GOING DIFFERENTIAL

- $1/\varepsilon^6$, $1/\varepsilon^5$, ... $1/\varepsilon^4$, $1/\varepsilon^3$, ... $1/\varepsilon^2$, $1/\varepsilon$
 - single unresolved
- single unresolved
- double unresolved

- single unresolved
- double unresolved
- triple unresolved

Projection-to-Born

- $gg \rightarrow H$ [Chen, Gehrmann, Glover, AH, Mistlberger, Pelloni '21] $q_{\rm T}$ subtraction • $gg \rightarrow H$
 - [Billis, Dehnadi, Ebert, Michel, Tackmann '21]
- $pp \rightarrow \gamma^*$

 $pp \rightarrow W$

[Chen, Gehrmann, Glover, AH, Yang, Zhu, '21]

 $pp \rightarrow Z$ [Camarda, Cieri, Ferrera '21] [NNLOJET + RadISH '22] [Neumann, Campbell '22]

[Chen, Gehrmann, Glover, AH, Yang, Zhu '22]

FULLY DIFFERENTIAL ggH @ N3LO

• only non-trivial observable:

• idea: restore *differential* info

projection to Born

[Chen, Gehrmann, Glover, AH, Mistlberger, Pelloni '21]

linear fiducial power corrections ⇒ instabilities

- can be cured
 by resummation

FULLY DIFFERENTIAL ggH @ N3LO

only non-trivial observable:

idea: restore differential info

projection to Born

[Chen, Gehrmann, Glover, AH, Mistlberger, Pelloni '21]

no instabilities & flat K-factor: $N^{3}LO \simeq NNLO \times K_{N^{3}LO}$

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qt SUBTRACTION @ N3LO

DRELL-YAN @ N3LO - Y_V DISTRIBUTIONS

same collider @ 13 TeV \rightarrow almost universal NNLO \rightarrow N³LO corrections! NC & CC[±] processes probe different parton content across Y_V (valence u vs. d, ...)

N3LO PARTON DISTRIBUTION FUNCTIONS

N3LO evolution ↔ 4-loop splitting functions

• aN3LO PDFs (MSHT)

ggH: $\delta \sigma^{N^3LO}$ VBF: $\delta \sigma^{N^3LO}$

CONCLUSIONS & OUTLOOK PART 1

- NNLO QCD calculations in good shape
 - $2 \rightarrow 2$ essentially solved
 - $2 \rightarrow 3$ new frontier $\leftrightarrow \rightarrow$ methods reaching maturity
 - *loop amplitudes* becoming a bottleneck again
 - in the quest for percent-level theory $\leftrightarrow \rightarrow$ mixed QCD×EW important
- dissemination of results
 - public codes (MCFM, Matrix), nTuples, ...
 - fast interpolation grids $\leftrightarrow APPLgrid fastNLO PineAPPL (anyway needed in fitting)$
- identified objects $\leftrightarrow \rightarrow$ mismatch in TH vs. Exp/NNLO
 - photon isolation, flavour tagging, hadron fragmentation, ...

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CONCLUSIONS & OUTLOOK PART 2

- N³LO predictions are key to reach percent-level accuracy
 - computation of *inclusive* $2 \rightarrow 1$ processes very mature $\iff ggH, DY, VBF, VH, \dots$
 - differential predictions for $pp \rightarrow$ "colour neutral" appearing ✓ relies on very stable NNLO "+jet" calculation
 - <u>*but:*</u> performance of slicing methods very poor $\leftrightarrow \delta$ (10M) CPU core hours
- Fiducial cuts \leftrightarrow linear power corrections (other processes?) \hookrightarrow crucial for practicability of slicing approaches
- Inadequacies in traditional scale variations \leftrightarrow DY @ N3LO \rightarrow effect from missing N³LO PDFs?
 - \rightarrow more robust TH uncertainties desirable

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Thank you!

