Pushing the multiplicity frontier of NNLO QCD predictions

Vasily Sotnikov
Max-Planck-Institute for Physics

based on
Dmitriy Chicherin, VS [JHEP 12 (2020) 167]
Samuel Abreu, Ben Page, Evgenij Pascual, VS [JHEP 21 (2020) 078]
Stefan Kallweit, Marius Wiesemann, VS [Phys. Lett. B 812 (2021) 136013]

INFN-UNIMI-UNIMIB Pheno Seminar (`Zoom` @ Milan)

9th March 2021

Outline

1. Introduction

2. Five-point two-loop amplitudes

   Transcendental part: pentagon functions

   Rational part: analytics from numerics

3. NNLO QCD predictions for triphoton production

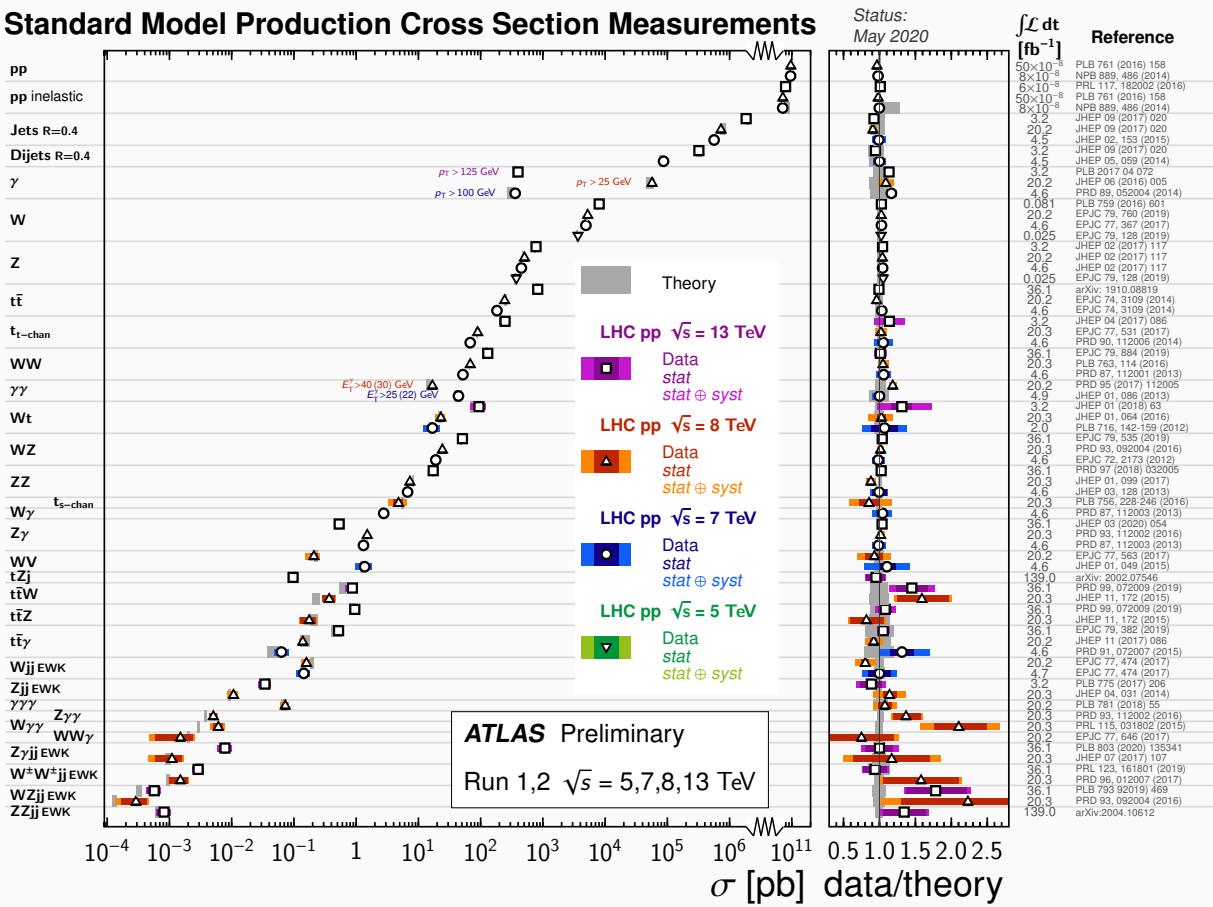
4. Conclusions & outlook

Introduction

Era of precision physics at the LHC

- LHC will still be running for years
- Many observables will be probed experimentally at $\sim$ percent level precision
- Discovery via precision: search anomalous deviations from Standard Model

[ATL-PHYS-PUB-2020-010]



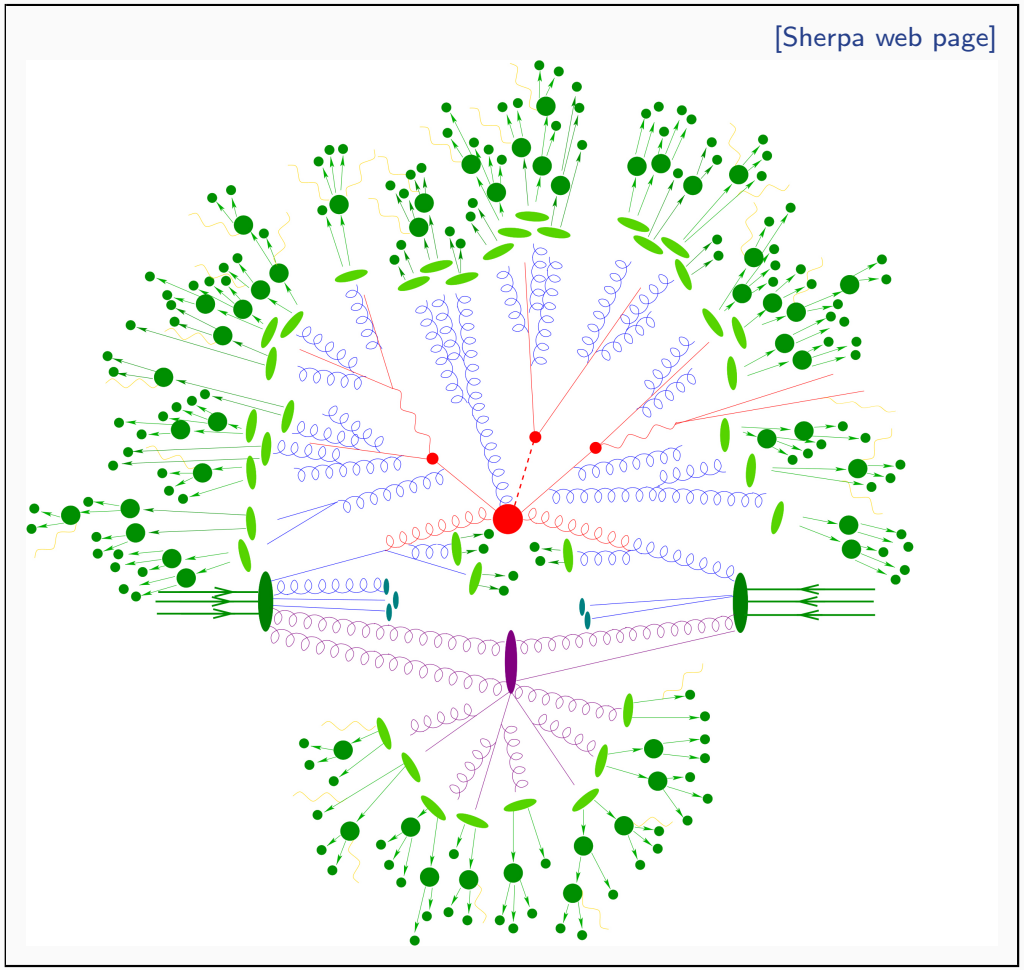
Theory must reach comparable precision target!

NNLO QCD and NLO EW computations generally required

(also NNLO PDFs, parton showers, resummation)

Proton collisions: a multi-layered process

[Sherpa web page]



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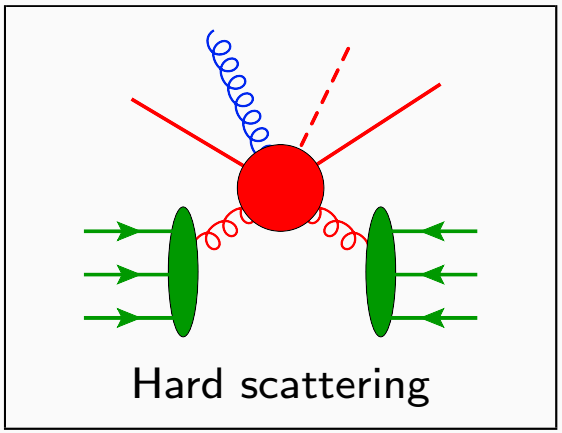
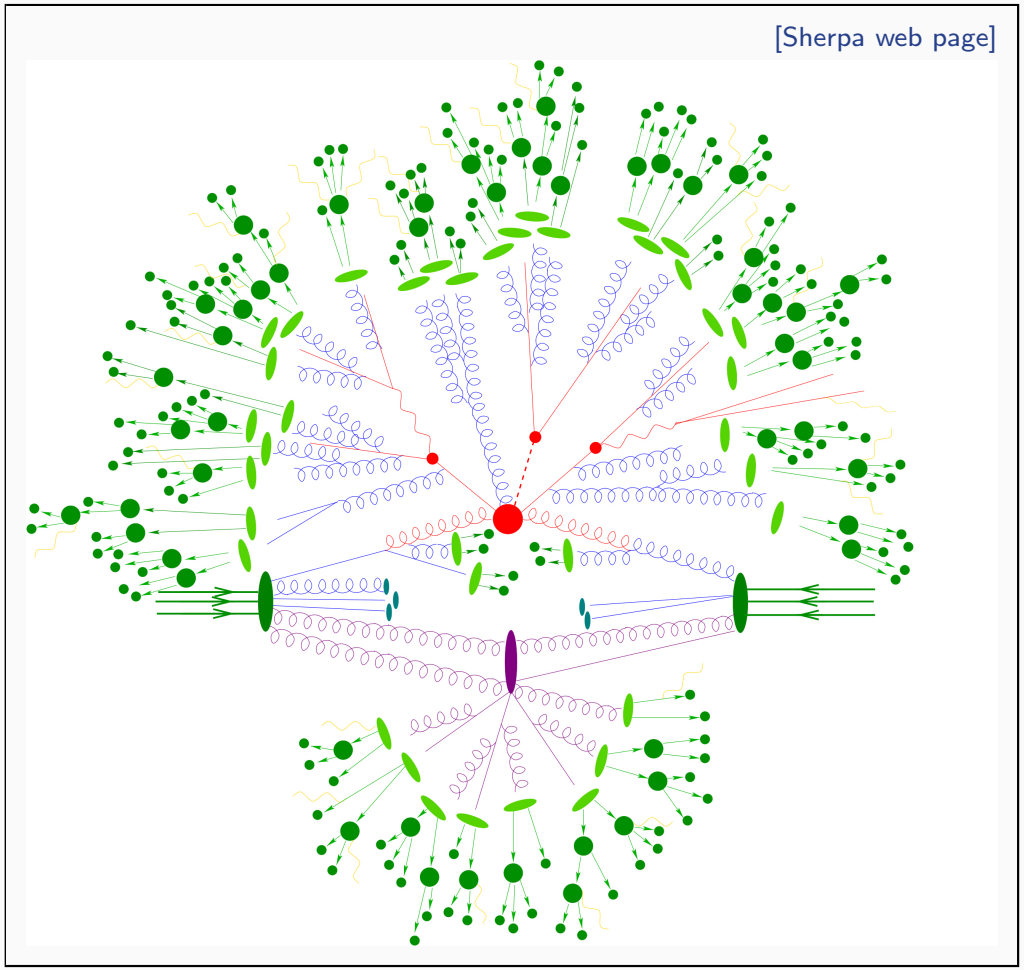
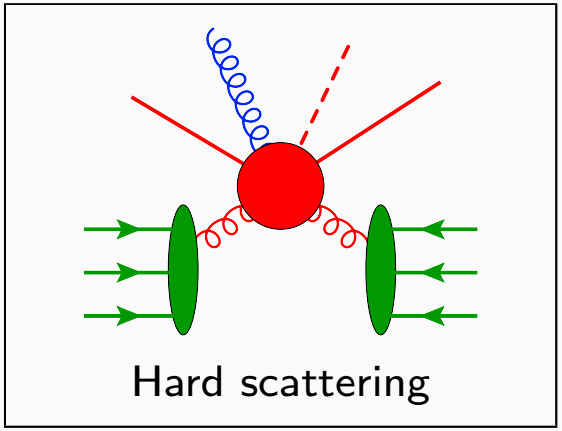


Proton collisions: a multi-layered process





$$\sigma \sim \overbrace{\underbrace{\sigma_{\text{LO}}\left(1+\alpha_s\sigma^{(1)}}_{\text{NLO}}+\alpha_s^2\sigma^{(2)}+\mathcal{O}\left(\alpha_s^3\right)\right)}^{\text{NNLO}}$$

naively $\lesssim 2\%$

NNLO QCD: Status

State of the art

- Many $2 \to 2$ NNLO QCD completed
- Next frontier is $2 \to 3$

Bottlenecks

- IR divergences
- Two-loop amplitudes

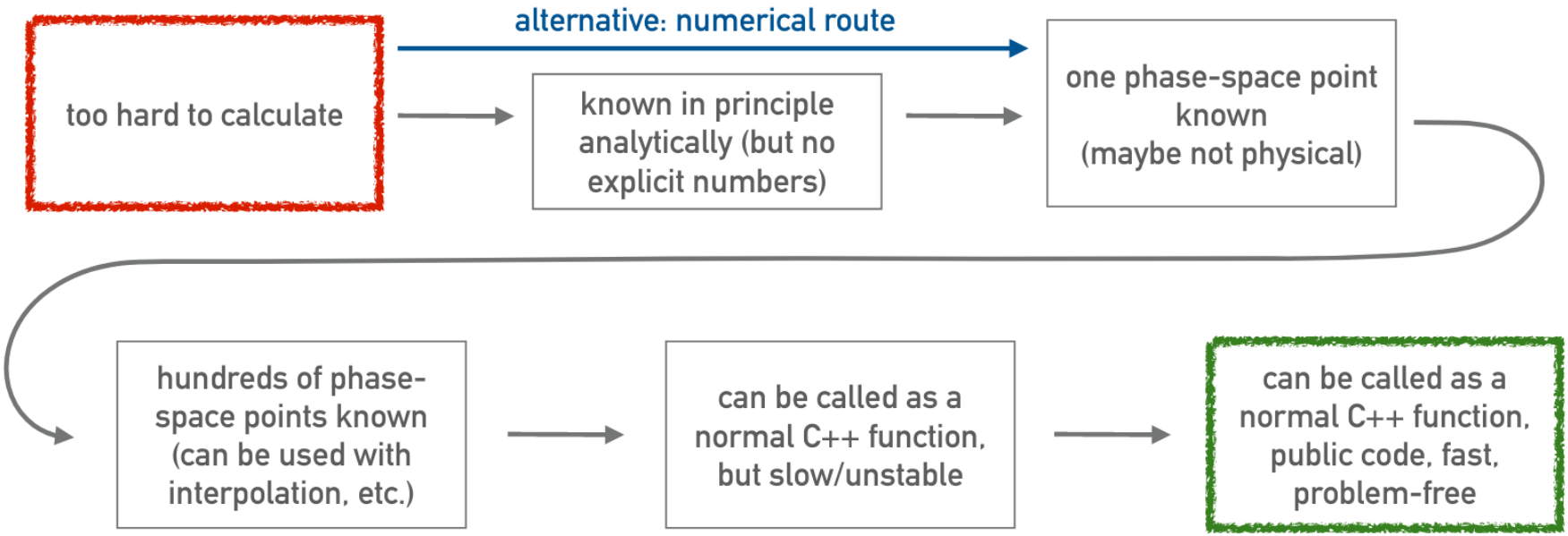
Les Houches wishlist 2019 [2003.01700]

process	known	desired
$pp \to 2\,\text{jets}$	NNLO_{QCD}	
	$\text{NLO}_{\text{QCD}} + \text{NLO}_{\text{EW}}$	
$pp \to 3\,\text{jets}$	$\text{NLO}_{\text{QCD}} + \text{NLO}_{\text{EW}}$	NNLO_{QCD} α_s running
⋮	⋮	⋮
$pp \to \gamma\gamma$	$\text{NNLO}_{\text{QCD}} + \text{NLO}_{\text{EW}}$	H p_T spectrum
$pp \to \gamma\gamma + j$	NLO_{QCD}	$\text{NNLO}_{\text{QCD}} + \text{NLO}_{\text{EW}}$
	NLO_{EW}	
$pp \to \gamma\gamma\gamma$	NNLO_{QCD}	anomalous gauge couplings
⋮	⋮	⋮
$pp \to V + j$	$\text{NNLO}_{\text{QCD}} + \text{NLO}_{\text{EW}}$	hadronic decays
		QCD precision physics
$pp \to V + 2j$	$\text{NLO}_{\text{QCD}} + \text{NLO}_{\text{EW}}$	NNLO_{QCD}
	NLO_{EW}	$H \to b\bar{b}$ decay
$pp \to V + b\bar{b}$	NLO_{QCD}	$\text{NNLO}_{\text{QCD}} + \text{NLO}_{\text{EW}}$
⋮	⋮	⋮
$pp \to H + 2j$	$\text{NLO}_{\text{HTL}} \otimes \text{LO}_{\text{QCD}}$	VBF studies
	$\text{N}^3\text{LO}_{\text{QCD}}^{(\text{VBF}^*)}$ (incl.)	$\text{NNLO}_{\text{HTL}} \otimes \text{NLO}_{\text{QCD}} + \text{NLO}_{\text{EW}}$
	$\text{NNLO}_{\text{QCD}}^{(\text{VBF}^*)}$	$\text{NNLO}_{\text{QCD}}^{(\text{VBF})} + \text{NLO}_{\text{EW}}^{(\text{VBF})}$
	$\text{NLO}_{\text{EW}}^{(\text{VBF})}$	

Five-point two-loop amplitudes

Stages of an amplitude

[Gavin Salam @ Zoomplitudes 2020]



Each stage brings important value.
For broad experimental use at the LHC,
we need to get to the last one (+ parton-shower matching etc.)

Five-point two-loop amplitudes: state of the art

Work on integrals

Massless [Papadopoulos, Tommasini, Wever '15] [Gehrmann, Henn, Lo Presti '18] [Abreu, Dixon, Herrmann, Page, Zeng '18] [Chicherin, Gehrmann, Henn, Wasser, Zhang, Zoia '18] [Abreu, Page, Zeng '18] [Chicherin, VS '20]
One external mass [Abreu, Ita, Moriello, Page, Tschernow, Zeng '20] [Canko, Papadopoulos, Syrrakos '20]

Work on two-loop amplitudes

[Gehrmann, Henn, Lo Presti '15] [Dunbar, Perkins '16] [Peraro '16] [Badger, Brønnum-Hansen, Hartanto, Peraro '18]

[Abreu, Febres Cordero, Ita, Page, VS '18] [Abreu, Dormans, Febres Cordero, Ita, Page '18]

[Abreu, Dormans, Febres Cordero, Ita, Page, VS '19]

[Badger, Chicherin, Gehrmann, Heinrich, Henn, Peraro, Wasser, Zhang, Zoia '19] [Abreu, Dixon, Herrmann, Page, Zeng '18]

[Chicherin, Gehrmann, Henn, Wasser, Zhang, Zoia '18] [Chawdry, Lim, Mitov '18] [Boels, Jin, Luo '18]

[Böhm, Georgoudis, Larsen, Schönemann, Zhang '18] [Wang, Li, Basat '19] [Guan, Liu, Ma '19]

[Chawdry, Czakon, Mitov, Poncelet '19] [Hartanto, Badger, Brønnum-Hansen '19] [Laurentis, Maître '20]

[Badger, Hartanto, Zoia '21], . . .

Phenomenology-ready results

$pp \to \gamma\gamma\gamma$	helicity, leading color	[Abreu, Page, Pascual, VS '20] [Chawdry, Czakon, Mitov, Poncelet '20]
$q\bar{q} \to \gamma\gamma g$	unpolarized, leading color	[Agarwal, Buccioni, von Manteuffel, Tancredi '21]
$q\bar{q} \to \gamma\gamma g$	helicity, leading color	[Chawdry, Czakon, Mitov, Poncelet '21]
$pp \to 3j$	helicity, leading color	[Abreu, Febres Cordero, Ita, Page, VS '21]

all rely on `PentagonFunctions++` [Chicherin, VS '20] for numerical evaluation

Anatomy of a loop amplitude

$$\mathcal{A} = \sum_{\mathbf{i}} r_{\mathbf{i}}(\vec{\mathbf{s}}, \epsilon)\ \mathbf{f}^{\mathbf{i}}(\vec{\mathbf{s}}, \epsilon)$$

rational (algebraic) part

transcendental part

- Process-dependent
- IBP reduction, finite-fields techniques, analytic reconstruction, numerical unitarity, etc.
- Evaluation time subleading if analytics known

- Depends only on kinematics
- No consensus on how to organize:
  master integrals?
  functions?
  what functions?
- Dominates evaluation time

Five-point two-loop amplitudes

Transcendental part: pentagon functions

The question

What is a good representation of transcendental part of two-loop multi-scale (≥ 5 legs) from phenomenological perspective?

Good =

1. Fast numerical evaluation with sufficient precision in all physical regions.
   evaluation of squared helicity/color summed amplitudes $\lesssim 1$min with precision $\gtrsim 2$ digits
2. Compact representation of rational (algebraic) coefficients
3. Manifest physical properties $\Longrightarrow$ numerical stability, singular limits

The solution

Understand well the underlying mathematical structures and be guided by them!

Feynman integrals: differential equations

If expressible through multiple polylogarithms (MPLs):

1. Find canonical DE [Henn '13] for integrals

$$\mathrm{d}\vec{f} = \epsilon \sum_i \mathrm{d}\log W_i \, A_i \, \vec{f} \qquad (\star)$$

Letters of "alphabet"

Rational matrix

2. Initial values from physical consistency conditions, etc.
3. Integrate $(\star)$ order-by-order in ϵ in terms of MPLs

MPLs well understood

- Relations and universal numerical evaluation.
- Extremely successful strategy for problems with few scales!

Difficulties in multi-scale cases

- Obtaining canonical DE nontrivial, still on case-by-case basis (not discussed here).
- Integrating ($\star$) ($\equiv$ explicit MPL solution) very challenging due to complicated algebraic letters.
  Some success with the *simplified differential equations* method [Papadopoulos '14] [Papadopoulos, Tommasini, Wever '15] [Canko, Papadopoulos, Syrrakos '20]
- Explosion of MPLs required to write the solution $\Longrightarrow$ unacceptably slow evaluation.
  Even the simplest case of five-point massless kinematics impractical!
- Analytic continuation

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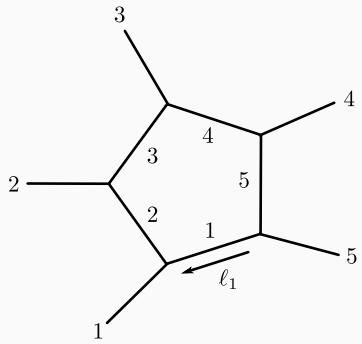
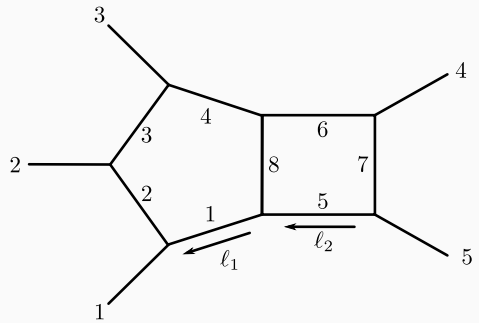
Iterated-integral based approach

- Construct minimal basis of transcendental functions from their iterated-integral representation [Gehrmann, Henn, Lo Presti '18] [Chicherin, VS '20]
- Manifest physical properties
- Dedicated numerical evaluation algorithms, not through MPLs

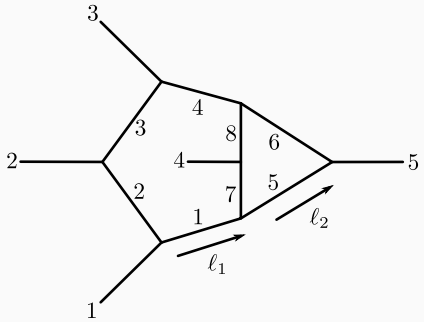
Integral topologies



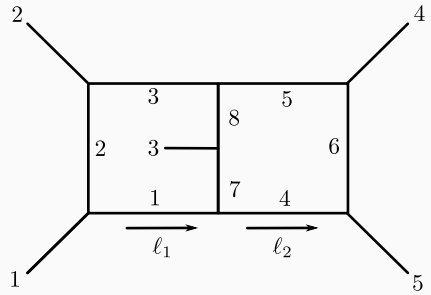
(P) pentagon



(a) (PB) planar pentagon-box



(HB) non-planar hexagon-box



(DP) non-planar double pentagon

τ	P	PB	HB	DP
# master integrals	$10\|1$	$53\|8$	$62\|11$	$88\|20$
# master integrals (top)	$0\|1$	$1\|2$	$1\|2$	$3\|6$

Differential equations

Bases of UT master integrals ($\Longleftrightarrow$ DE in canonical form) known for all 4 topologies

[Gehrmann, Henn, Lo Presti '18] [Chicherin, Gehrmann, Henn, Lo Presti, Mitev, Wasser '18]

[Chicherin, Gehrmann, Henn, Wasser, Zhang, Zoia '18] [Abreu, Dixon, Herrmann, Page, Zeng '18] [Abreu, Page, Zeng '18]

$$\mathrm{d}\vec{f}_{\tau,\sigma} = \epsilon\, \mathrm{d}\tilde{A}_{\tau,\sigma}\, \vec{f}_{\tau,\sigma},$$

$$\mathrm{d}\tilde{A}_{\tau,\sigma} = \sum_{i=1}^{31} a^{(i)}_{\tau,\sigma}\, \mathrm{d}\log W_i$$

- $5!$ permutations $\sigma \in \mathcal{S}_5$ for each topology
- single initial point in physical region
  $X_0 : (v_1, v_2, v_3, v_4, v_5) = (3, -1, 1, 1, -1)$
  $\epsilon_5 = \mathrm{i}\sqrt{3}$

$\Longleftrightarrow$ no analytic continuation needed

Iterated integrals

[Chen '77] (see also *"Iterated integrals in QFT"* [Brown '11])

Let $\omega_1, \ldots, \omega_n$ be differential 1-forms on $M (\boldsymbol{s} \in M)$, and path $\gamma : [0,1] \to M$. Denote the pull-back of the forms ω_i as $\gamma^\star \circ \omega_i = w_i(t)\,\mathrm{d}t$

$$I_\gamma[\omega_1, \ldots, \omega_n] = \int_0^1 w_n(t_n)\,\mathrm{d}t_n \ldots \int_0^{t_2} w_1(t_1)\,\mathrm{d}t_1 \tag{ii}$$

For logarithms forms $\omega_i = \mathrm{d}\log(W_i)$ we use notation

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Shuffle product

$$I_\gamma[\omega_1, \ldots, \omega_r]\; I_\gamma[\omega_{r+1}, \ldots, \omega_n] = \sum_{\boldsymbol{i} \in \{1,\ldots,r\} \sqcup\!\sqcup \{r+1,n\}} I_\gamma[\omega_{i_1}, \ldots, \omega_{i_n}] \tag{ш}$$

Given independent integration kernels,

- linearize polynomial identities
- only trivial linear combinations vanish

Classification strategy

[Chicherin, VS '20] (partially introduced in [Gehrmann, Henn, Lo Presti '18])

Goal: construct complete set of algebraically independent transcendental functions

- Rely only on properties of iintegrals
- Proceed iteratively order-by-order in ϵ (or transcendental weight w)

Assume $\boldsymbol{g}^{(w-1)}$, a set of functions for weight $w-1$, is known. At weight w,

1. Solve $4 \times 5!$ DEs in terms of iintegrals (trivial)

$$\vec{f}^{(w)} = \sum_{w'=0}^{w} \sum_{i_1,\ldots,i_{w'}=1}^{31} \vec{\kappa}^{(w-w')}_{i_1,\ldots,i_{w'}} \left[W_{i_1},\ldots,W_{i_{w'}}\right]_{X_0}$$

   Master integrals $\vec{f}$ in $\mathbb{Q}$-linear span of iintegrals (and constants κ)

2. Add products of $\boldsymbol{g}^{(w'<w)}$ and use shuffle algebra to put into same vector space
3. Find basis of combined linear span, preferring lower-weight products $\Longrightarrow$ irreducible iintegrals $\boldsymbol{g}^{(w)}$

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master integrals	30360
topologically independent	1917

	1	2	3	4
iintegrals (symbols)	10	79	482	1462
irreducible iintegrals	10	24	111	472

Weights 1 and 2: Li_2 representation

Convenient to choose a basis of explicit $\log$ and Li_2 functions instead of iintegrals themselves.

For example,

$$g^{(1)}_{1,4} = \log(s_{45}) = [W_4]$$

$$g^{(1)}_{2,10} = \log\left(\sqrt{\Delta}\right) = [W_{31}] + \frac{\mathrm{i}\,\pi}{2} + \frac{\log(3)}{2}$$

$$g^{(2)}_{2,1} = \mathrm{Li}_2\left(\frac{1}{W_{27}}\right) - \mathrm{Li}_2\left(W_{27}\right) + \mathrm{Li}_2\left(\frac{1}{W_{28}}\right) - \mathrm{Li}_2\left(W_{28}\right) - \mathrm{Li}_2\left(\frac{1}{W_{27}W_{28}}\right) + \mathrm{Li}_2\left(W_{27}W_{28}\right) =$$

$$-[W_1,W_{27}] - [W_1,W_{28}] - [W_2,W_{27}] - [W_2,W_{28}] + [W_3,W_{27}] + [W_5,W_{28}] +$$
$$[W_{18},W_{28}] + [W_{19},W_{27}] - [W_{27}]\log(3) - [W_{28}]\log(3) + \frac{8\,\mathrm{i}}{3}\,\mathrm{Im}\,\mathrm{Li}_2\left(\frac{1}{2} + \frac{\mathrm{i}\sqrt{3}}{2}\right)$$

Weight 3: one-fold integral representation

Weight 3 functions are one-fold integrals of weight 2 functions by definition

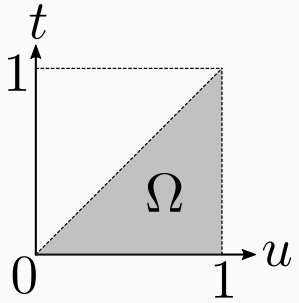
$$g_i^{(3)} = \sum_{j=1}^{31} \int_\gamma \mathrm{d}\log W_j \, h_{i,j}^{(2)}$$

Integrands analytic on the integration domain $\implies$ integration well-defined.

Weight 4: one-fold integral representation

Change order of integration [Caron-Huot, Henn '14]

$$I_\gamma[\omega_1,\ldots,\omega_n] =$$
$$\int_0^1 (\gamma^\star\circ\omega_n)(t)\int_0^t (\gamma^\star\circ\omega_{n-1})(u)\; I_{\gamma(u)}[\omega_1,\ldots,\omega_{n-2}]$$
$$= \int_0^1 (\gamma^\star\circ\omega_{n-1})(u)\left(\int_u^1 (\gamma^\star\circ\omega_n)(t)\right)\; I_{\gamma(u)}[\omega_1,\ldots,\omega_{n-2}]$$



For logarithmic forms the last integration is trivial

$$\int_u^1 (\gamma^\star\circ\omega_n)(t) = \int_u^1 \mathrm{d}\log\left(W_n(t)\right) = \log(W_n(1)) - \log(W_n(u))$$

Integrands are analytic, except possibly at the endpoint $u=0$, where integrable logarithmic divergences can occur

Numerical evaluation

Implemented in C++ library

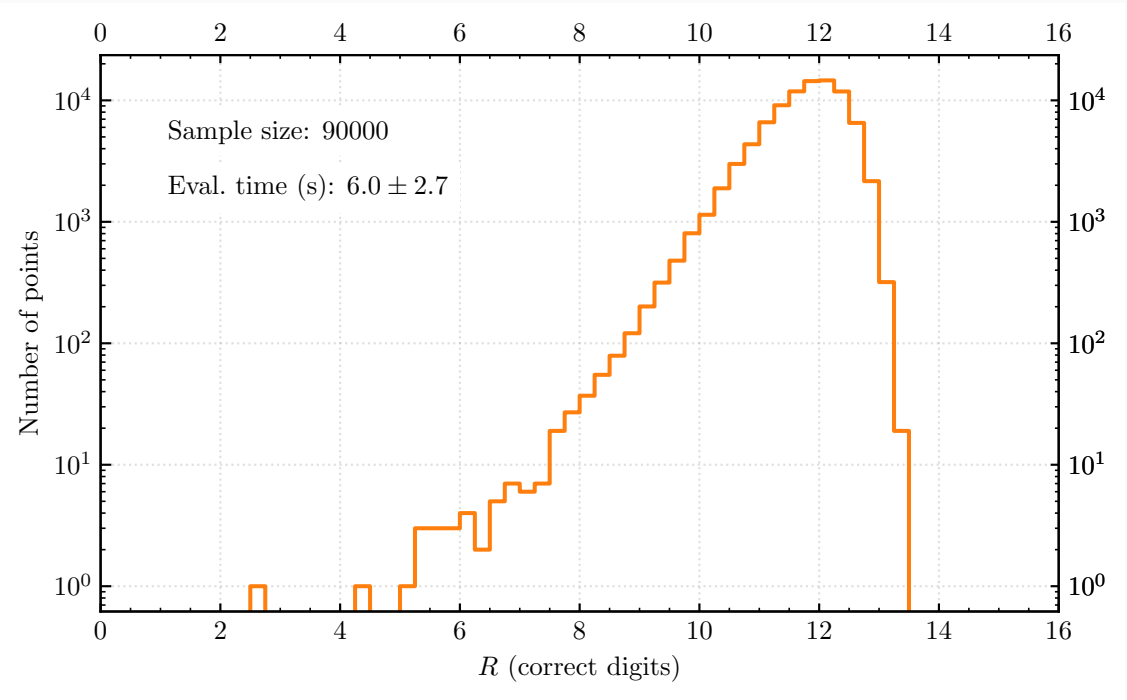
https://gitlab.com/pentagon-functions/PentagonFunctions-cpp

- Li_2 and Cl_2 evaluated with C++ library Li2++
- One-fold integrals numerically with double-exponential *tanh-sinh* quadrature [Takahasi, Mori '73]
- Quadruple and octuple precision available

Performance

Evaluate all functions:
any massless
five-point amplitude
in all "crossings"

Sampled over physical
phase-space for
$pp \to \gamma\gamma\gamma$



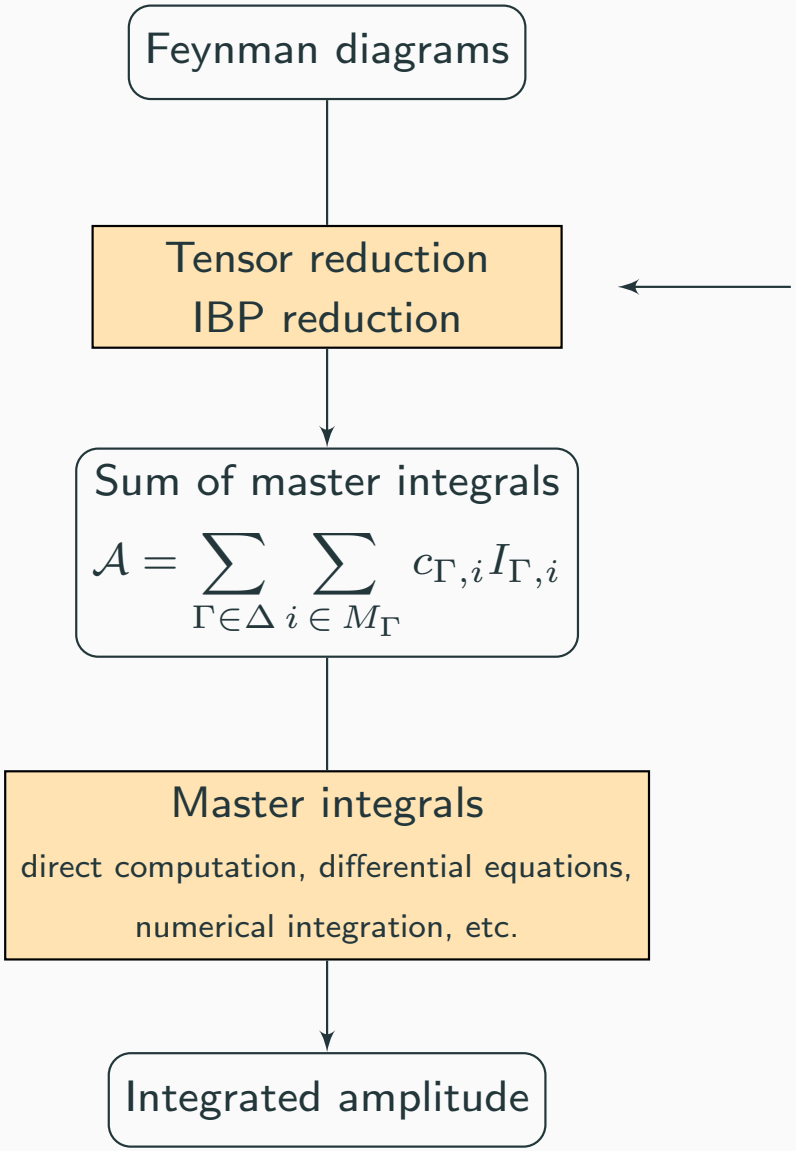
(vs. quad precision targets)

[Chicherin, VS '20]

Five-point two-loop amplitudes

Rational part: analytics from numerics

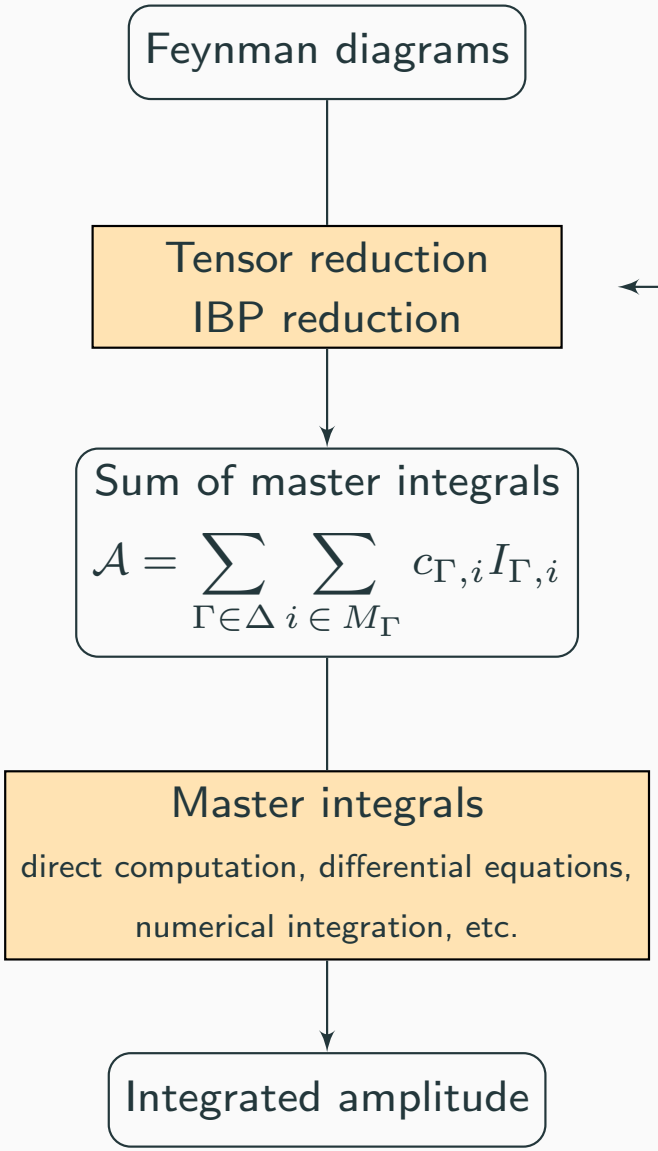
"Standard" approach



Challenges

- Large intermediate expressions
- Analytic IBP reduction tables are hard to get and to use (e.g. size 22 GB)
  [Boels, Jin, Luo '18] [Chawdhry, Lim, Mitov '18]
  (but good progress with finite fields recently)

"Standard" approach



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try to avoid these with

Numerical unitarity method

- No need to solve large IBP systems
- Numerical framework:
  less sensitive to addition of scales
- Targeted reconstruction of analytics:
  get final compact results directly from numerical samples

Numerical unitarity: universal ansatz

Build ansatz for integrand of full amplitude:

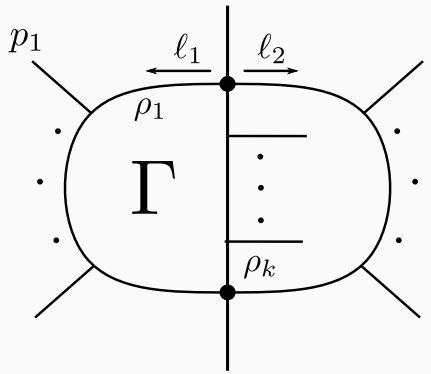
$$\mathcal{A}(\ell_l) = \sum_{\Gamma} \sum_{i \in M_\Gamma \cup S_\Gamma} c_{\Gamma,i} \, \frac{m_{\Gamma,i}(\ell_l)}{\prod_{j \in P_\Gamma} \rho_j}$$

Master terms

coefficients of master integrals

Surface terms

vanish upon loop integration



Generalization of one-loop unitarity methods:

[Bern, Dixon, Kosower, Dunbar '94, '95] [Britto, Feng, Cachazo '05] [Ossola, Papadopoulos, Pittau '07]

[Ellis, Giele, Kunszt '08] [Giele, Kunszt, Melnikov '08]

Related work

[Badger, Frellesvig, Zhang '12] [Zhang '12] [Mastrolia, Mirabella, Ossola, Peraro '13]

[Ita '15] [Mastrolia, Peraro, Primo '16] [Abreu, Febres Cordero, Ita, Jaquier, Page, Zeng '17]

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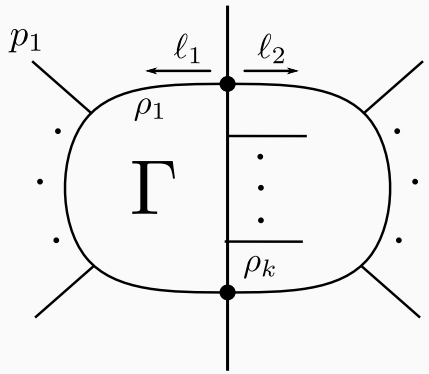
vanish upon loop integration



Surface terms produced from unitarity-compatible IBPs [Gluza, Kadja, Kosower '11]:

$$\int \left(\prod_l \mathrm{d}^D \ell_l \right) \sum_l \frac{\partial}{\partial \ell_l^\nu} \left(\frac{u_l^\nu \, \boldsymbol{\alpha}^{\vec{\mathbf{i}}}}{\prod_{j \in P_\Gamma} \rho_j} \right) = 0, \qquad u_l^\nu \frac{\partial}{\partial \ell_l^\nu} \rho_j = f_j \rho_j$$

- Find generating IBP vectors employing computational algebraic geometry methods (e.g. Singular) [Abreu, Febres Cordero, Ita, Page, Zeng '17] [Ita '15] [Larsen, Zhang '15] [Georgoudis, Larsen, Zhang '16]
- Choose any master terms from $\mathrm{span}\{\boldsymbol{\alpha}^{\vec{\mathbf{i}}}\} \setminus S_\Gamma$

Process-dependence contained in coefficients $c_{\Gamma,i}$ only

Numerical unitarity: cut equations

Obtain coefficients $c_{\Gamma,i}$ from linear systems of cut equations:

topologies with more propagators

$$\lim_{\ell_l \to \ell_l^\Gamma} \left(\mathcal{A}(\ell_l) \prod_{j \in P_\Gamma} \rho_j \right) = \sum_i c_{\Gamma,i}\, m_{\Gamma,i} + \sum_{\Gamma' > \Gamma} \sum_i c_{\Gamma',i} \frac{m_{\Gamma',i}}{\prod_{j \in P_{\Gamma'} \setminus P_\Gamma} \rho_j},$$

on-shell limit for Γ

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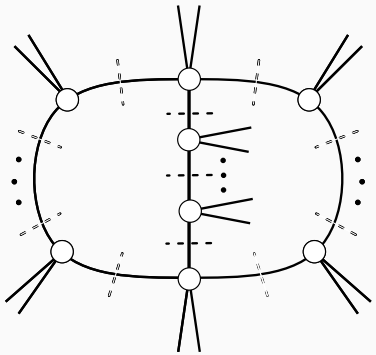
on-shell limit for Γ

$\Big\|$ Unitarity $\to$ factorization into product of trees



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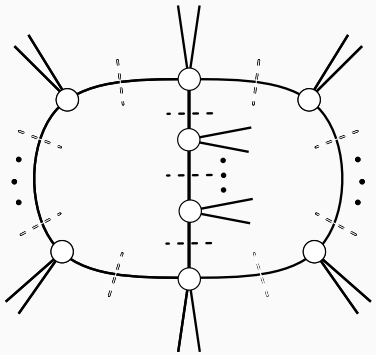
Unitarity $\to$ factorization into product of trees

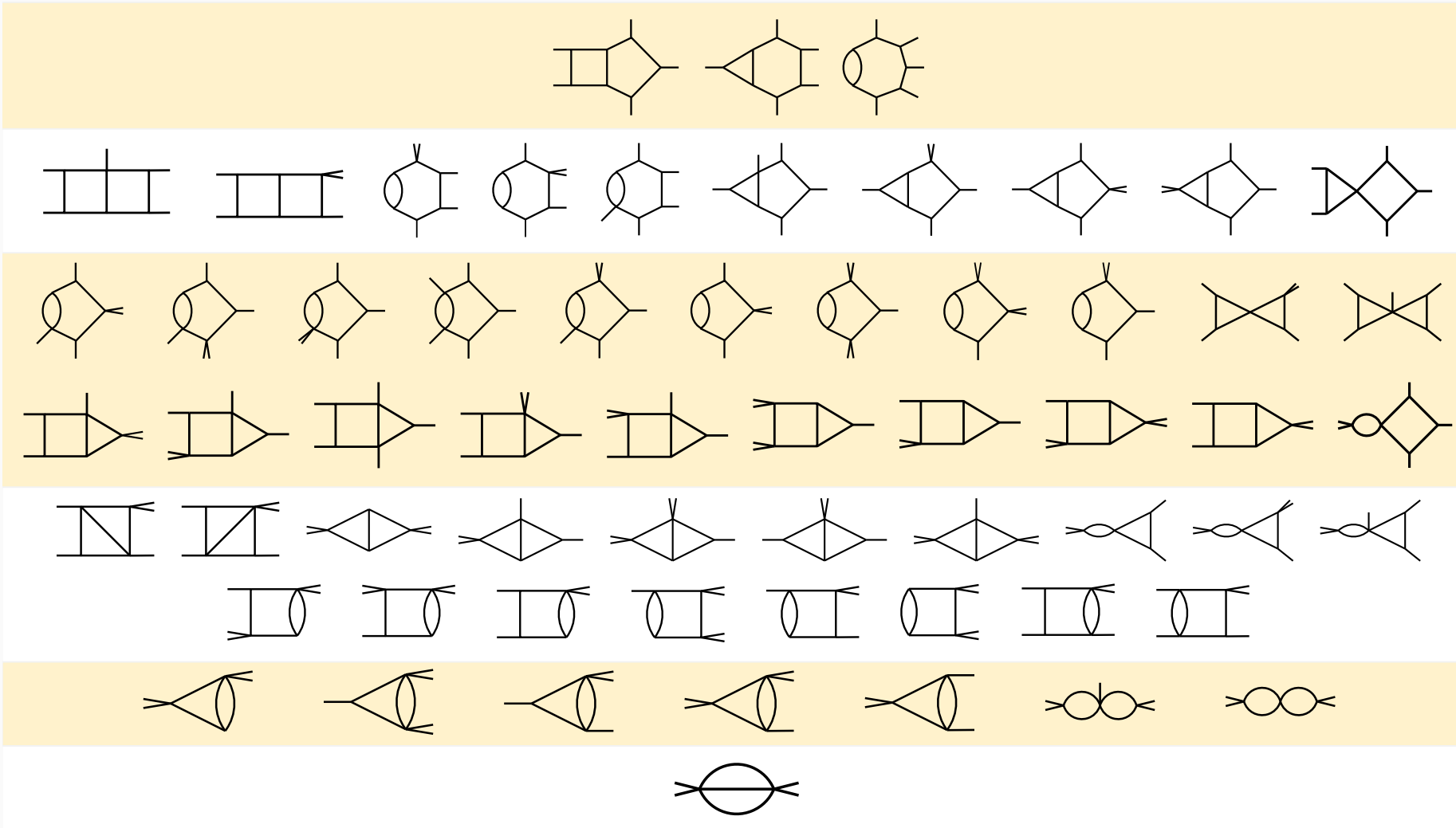


1. Sample ℓ_l^Γ to generate equations
2. Evaluate LHS with Berends-Giele off-shell recursion
3. Solve with standard linear algebra (PLU, QR, etc.)
4. Top to bottom, *recycle* coefficients:
   one topology at a time

Solve cut equations numerically!

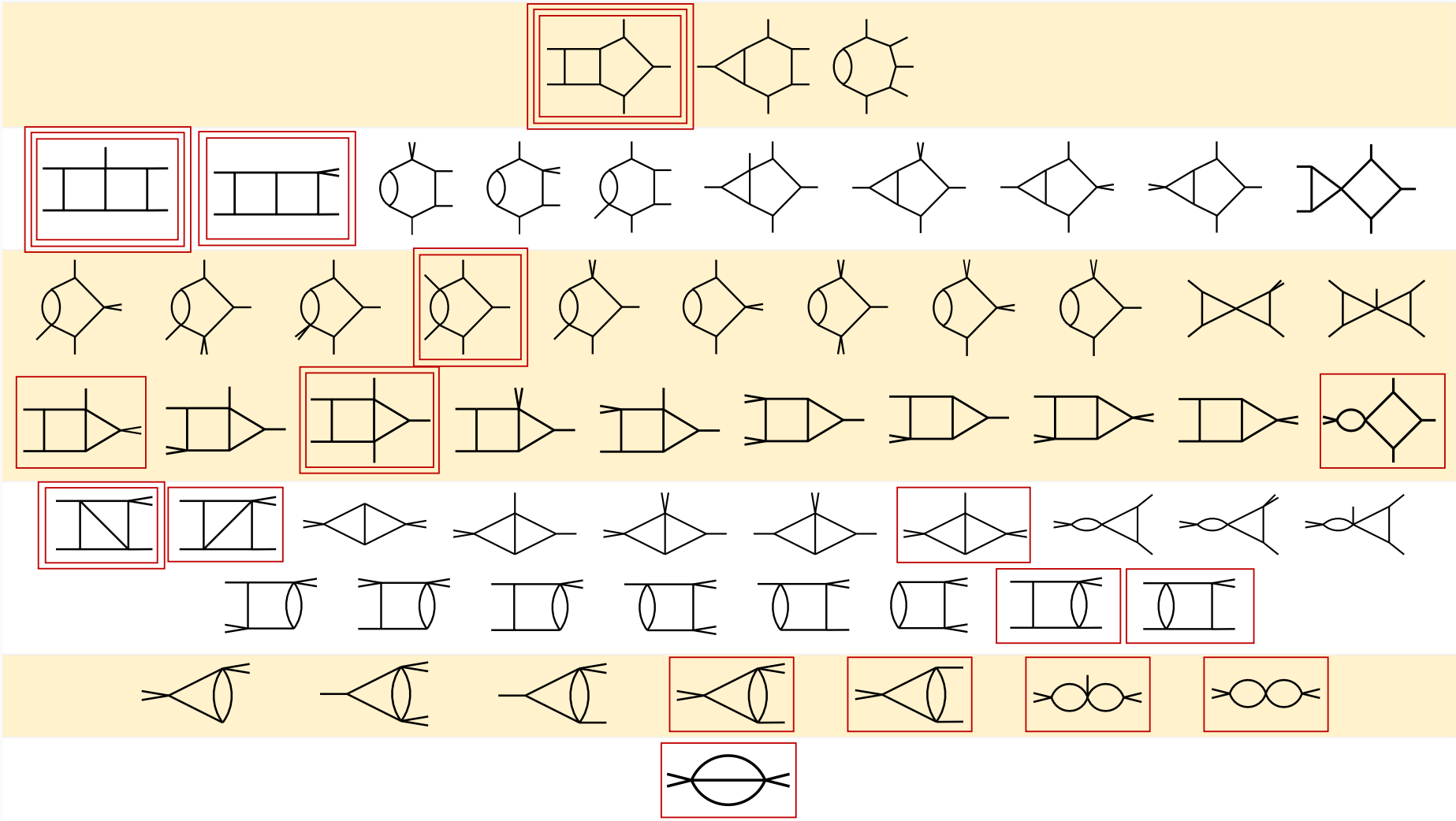
- no need to know analytic integrand
- suitable for floating point and finite fields

Topologies for five-point amplitudes



Full hierarchy (mod permutations)

Topologies for five-point amplitudes



Master integrals (mod permutations)

Analytic results from finite-field evaluations

Numerical unitarity

$$\mathcal{A} = \sum_{\Gamma \in \Delta} \sum_{i \in M_\Gamma} c_{\Gamma,i}(\mathbf{x}, \epsilon)\, \mathcal{I}_{\Gamma,i} \qquad c_{\Gamma,i}(\mathbf{x}) = \frac{\sum_{\vec{\mathbf{j}}} n_{\Gamma,i;\vec{\mathbf{j}}}\, \mathbf{x}^{\vec{\mathbf{j}}}}{\sum_{\vec{\mathbf{j}}} d_{\Gamma,i;\vec{\mathbf{j}}}\, \mathbf{x}^{\vec{\mathbf{j}}}},$$

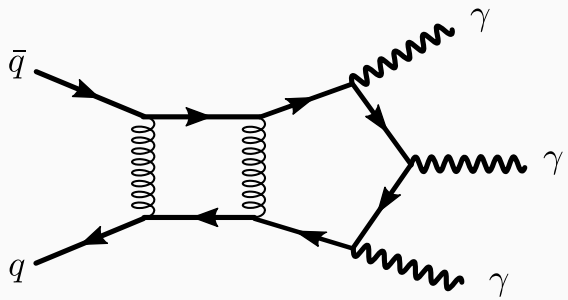
- Master-integral coefficients are rational functions of external kinematics
- Sample enough number of times (over finite fields) $\Longrightarrow$ relations for $n_{\Gamma,i;\vec{\mathbf{j}}}$, $d_{\Gamma,i;\vec{\mathbf{j}}}$ $\Longrightarrow$ analytics [von Manteuffel, Schabinger '14] [Peraro '16]

Efficient general purpose reconstruction algorithms now available:
`FireFly` [Klappert, Lange '19], `FiniteFlow` [Peraro '19]

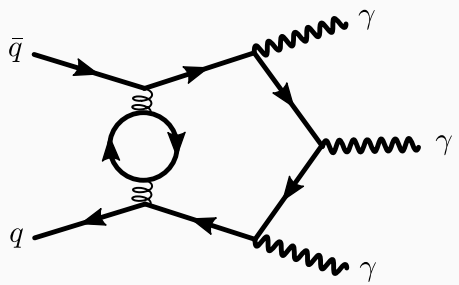
However

- Amplitudes are not random rational functions, analytic structure constrained by physical properties
- Can seriously simplify reconstruction by judicious ansatzing
  [Abreu, Dormans, Febres Cordero, Ita, Page, VS '19]

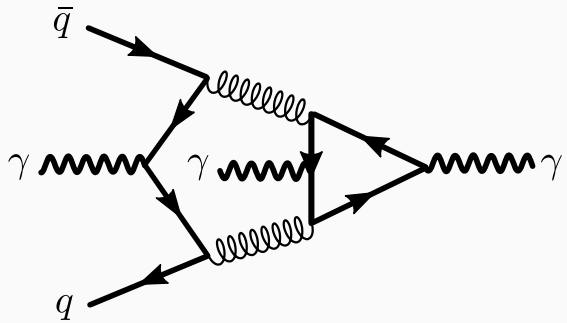
$q\bar{q} \to \gamma\gamma\gamma$ two-loop helicity amplitudes



$A^{(2,0)}$



$A^{(2,N_\mathrm{f})}$



$A^{(2,\tilde{N}_\mathrm{f})}$

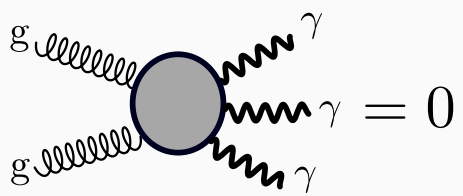
$$\mathcal{A}^{(1)} = C_F A^{(1)}$$

$$\mathcal{A}^{(2)} = C_F^2 B^{(2,0)} + C_F C_A B^{(2,1)} + C_F T_F N_\mathrm{f} A^{(2,N_\mathrm{f})} + C_F T_F \left(\sum_{f=1}^{N_\mathrm{f}} Q_f^2 \right) A^{(2,\tilde{N}_\mathrm{f})}$$

$$\xrightarrow{\mathsf{LC}} \frac{N_c^2}{4} \left(A^{(2,0)} + \mathcal{O}(N_\mathrm{c}^{-2}) \right) + C_F T_F N_\mathrm{f} \, A^{(2,N_\mathrm{f})}$$

2 helicity configurations:

$q^+\bar{q}^- \to \gamma^+\gamma^+\gamma^+$
$q^+\bar{q}^- \to \gamma^-\gamma^+\gamma^+$



Analytic results

[Abreu, Page, Pascual, VS '20]

Analytic results for finite remainders (UV/IR-renormalized amplitudes) expressed in pentagon functions

$$\mathcal{R}^{(2)} = \mathcal{A}^{(2)} - \mathbf{I}^{(1)}\mathcal{A}^{(1)} - \mathbf{I}^{(2)}\mathcal{A}^{(0)} = \sum_{\vec{\mathbf{i}}} r_{\vec{\mathbf{i}}}(\vec{\boldsymbol{s}})\, \boldsymbol{g}^{\vec{\mathbf{i}}},$$

$$\boldsymbol{g}^{\vec{\mathbf{i}}} = g_1^{i_1} \cdots g_n^{i_n}, \qquad \sum_k \text{weight}(g_k^{i_k}) \leq 4$$

from exact numerical evaluations with Caravel

[Abreu, Dormans, Febres Cordero, Ita, Kraus, Page, Pascual, Ruf, VS '20]

- 4 min per finite-field evaluation
- Needed 46k sample points to reconstruct analytic results

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- 4 min per finite-field evaluation
- Needed 46k sample points to reconstruct analytic results

Functions $r_{\vec{\mathbf{i}}}$ have nice analytic structure

$\Longrightarrow$ multivariate partial fractions

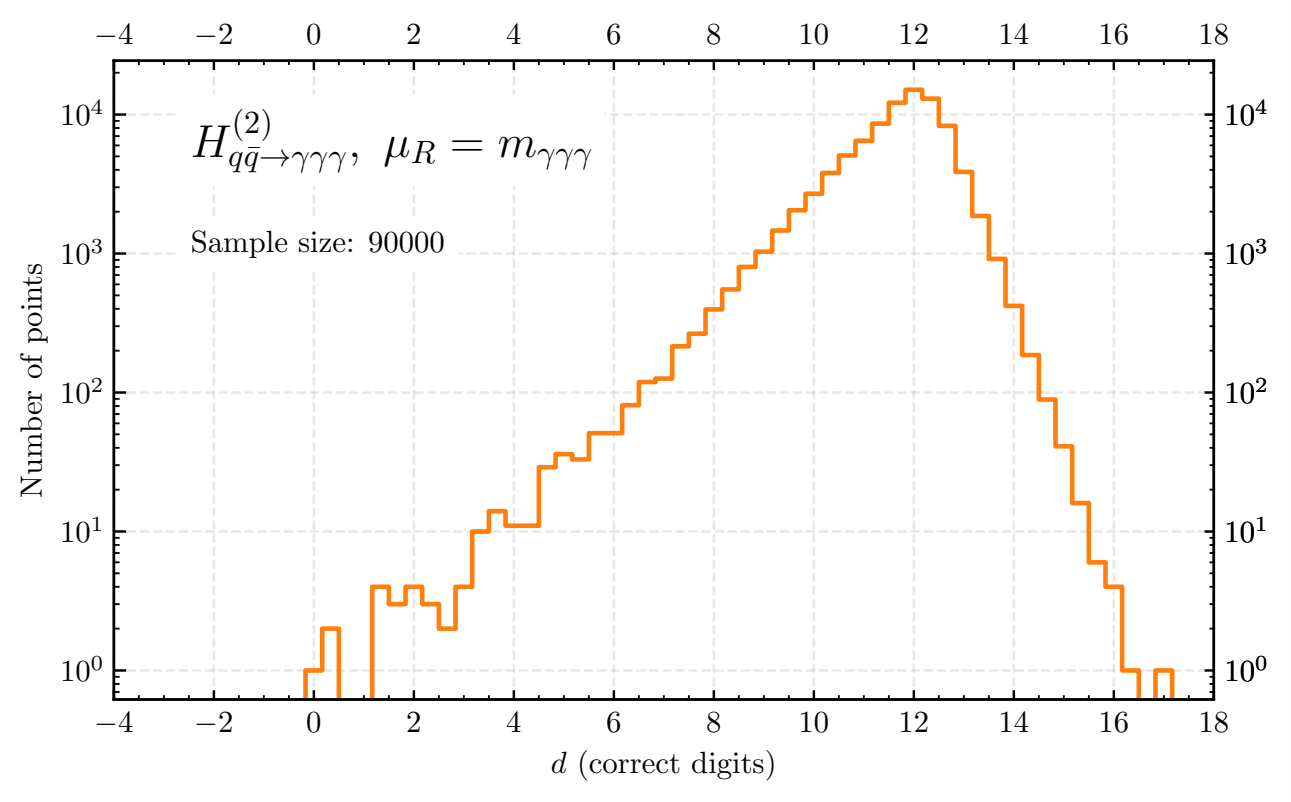
[Abreu, Dormans, Febres Cordero, Ita, Page, VS '19] (see also [Heller, von Manteuffel '21])

$\Longrightarrow$ compact analytic result, total size 1.5 Mb

Numerical evaluation

Available in C++ library:
https://gitlab.com/five-point-amplitudes/FivePointAmplitudes-cpp

- excellent stability
- $\sim$ 1s per phase-space point
- 96% spent on pentagon functions



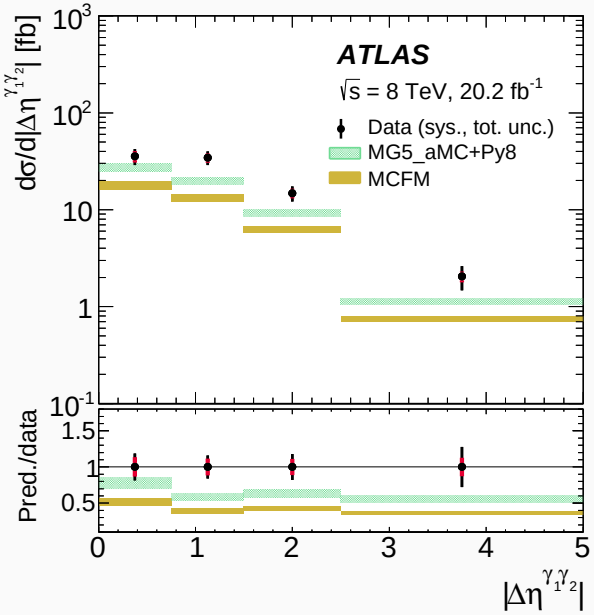
Numerical stability
(vs. quad precision targets)

[Abreu, Page, Pascual, VS '20]

NNLO QCD predictions for triphoton production

Motivation

- Previous tensions between NLO QCD predictions and 8 TeV measurements [arXiv:1712.07291]
- Main irreducible background for anomalous quartic gauge and anomalous Higgs couplings
- Slow perturbative convergence



Already studied in [Chawdry, Czakon, Mitov, Poncelet '19] within STRIPPER framework [Czakon '10,'11], but

- Very challenging, the first NNLO QCD $2 \to 3$ computation $\implies$ independent calculation important
- Fully flexible and publicly available results to allow follow-up studies

q_T subtraction (slicing)

$$h_1 + h_2 \to F + X$$

[Catani, Grazzini '07]

q_T — transverse momentum of color singlet system F, $\quad r = \frac{q_T}{m_F}$

$q_T = 0$ in LO kinematics

$$\sigma^F_{\mathrm{NNLO}} = \int_{\Phi_F} \mathrm{d}\sigma_{\mathrm{B}} + \int_{\Phi_F} \mathrm{d}\sigma_{\mathrm{V}} + \int_{\Phi_{F+1}} \mathrm{d}\sigma_{\mathrm{R}} + \int_{\Phi_{F+2}} \mathrm{d}\sigma_{\mathrm{RR}} + \int_{\Phi_{F+1}} \mathrm{d}\sigma_{\mathrm{RV}} + \int_{\Phi_F} \mathrm{d}\sigma_{\mathrm{VV}}$$

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$$\mathrm{d}\sigma^{\text{F}}_{\text{NNLO}} = \mathcal{H}_{\text{NNLO}} \otimes \mathrm{d}\sigma_{\text{B}} \; + \; \left(\mathrm{d}\sigma^{F+\text{jet}}_{\text{NLO}} - \mathrm{d}\sigma^{\text{CT}}_{\text{NNLO}}\right)$$

$\mathrm{d}\sigma^{F+\text{jet}}_{\text{NLO}}$ finite with $r > 0 \implies$ Catani-Seymour calculation [Catani, Seymour '96 '97]

$\mathrm{d}\sigma^{\text{CT}}_{\text{NNLO}}$ universal counterterm, known from small q_T resummation [Bozzi, Catani, de Florian, Grazzini '05]

$\mathcal{H}_{\text{NNLO}}$ particular IR renormalization of loop corrections [Catani, Cieri, de Florian, Ferrera, Grazzini '13]

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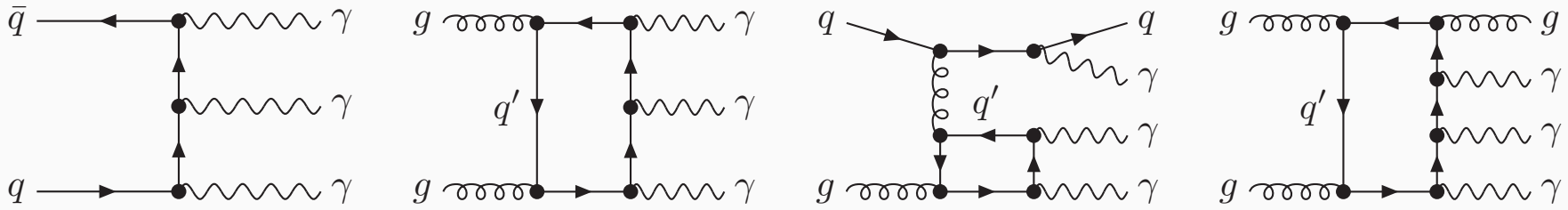
$r_{\text{cut}} \to 0$ extrapolation automated in MATRIX [Grazzini, Kallweit, Wiesemann '17]



$= 0$ finite, small $\lesssim 1\%$

- Phase space integration, NLO Catani-Seymour, q_T-subtraction within MATRIX [Grazzini, Kallweit, Wiesemann '17]
- Tree-level, one-loop from OpenLoops [Cascioli, Maierhöfer, Pozzorini '11]
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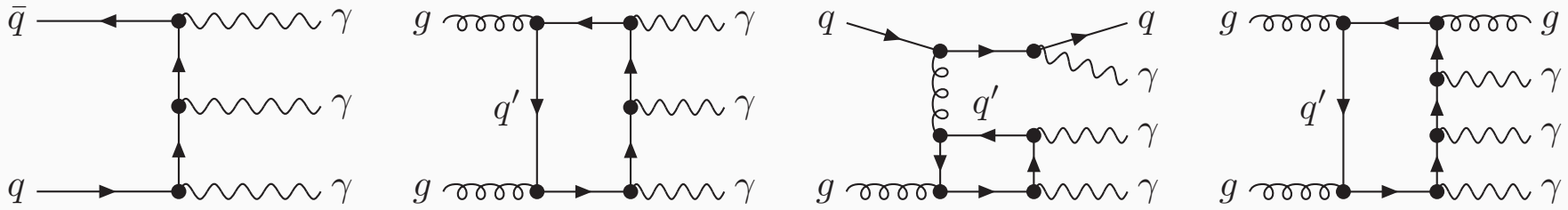

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- $\mathcal{H}^{(2,1)}$, $\mathcal{H}^{(2,\tilde{N}_\mathrm{f})}$ include non-planar two-loop contributions (difficult, WIP)
- $\mathcal{H}^{(2,N_\mathrm{f})}$, $\mathcal{H}^{(2,\tilde{N}_\mathrm{f})}$ contributions expected numerically subleading [Kallweit, VS, Wiesemann '20]

Phase space and parameters

$\sqrt{s} = 7, 8, 13, 14, 27, 100$ TeV
G_μ scheme for the EW parameters, $\alpha_s(m_Z) = 0.118$, NNPDF3.1

Fiducial phase space from ATLAS 8 TeV analysis [arXiv:1712.07291]:

- $p_{T,\gamma_1} \geq 27\,\text{GeV}$, $p_{T,\gamma_2} \geq 22\,\text{GeV}$, $p_{T,\gamma_3} \geq 15\,\text{GeV}$,
- $0 \leq |\eta_\gamma| \leq 1.37$ or $1.56 \leq |\eta_\gamma| \leq 2.37$, $m_{\gamma\gamma\gamma} \geq 50$
- Separated photons $\Delta R_{\gamma\gamma} \geq 0.45$
- Remove fragmentation photons: Frixione isolation [Frixione '98] with $n = 1$, $\delta_0 = 0.4$, and $E_T^{\text{ref}} = 10\,\text{GeV}$

Dynamical central scale $\mu_R = \mu_F = \frac{1}{4}\left(p_{T,\gamma_1} + p_{T,\gamma_2} + p_{T,\gamma_3}\right)$

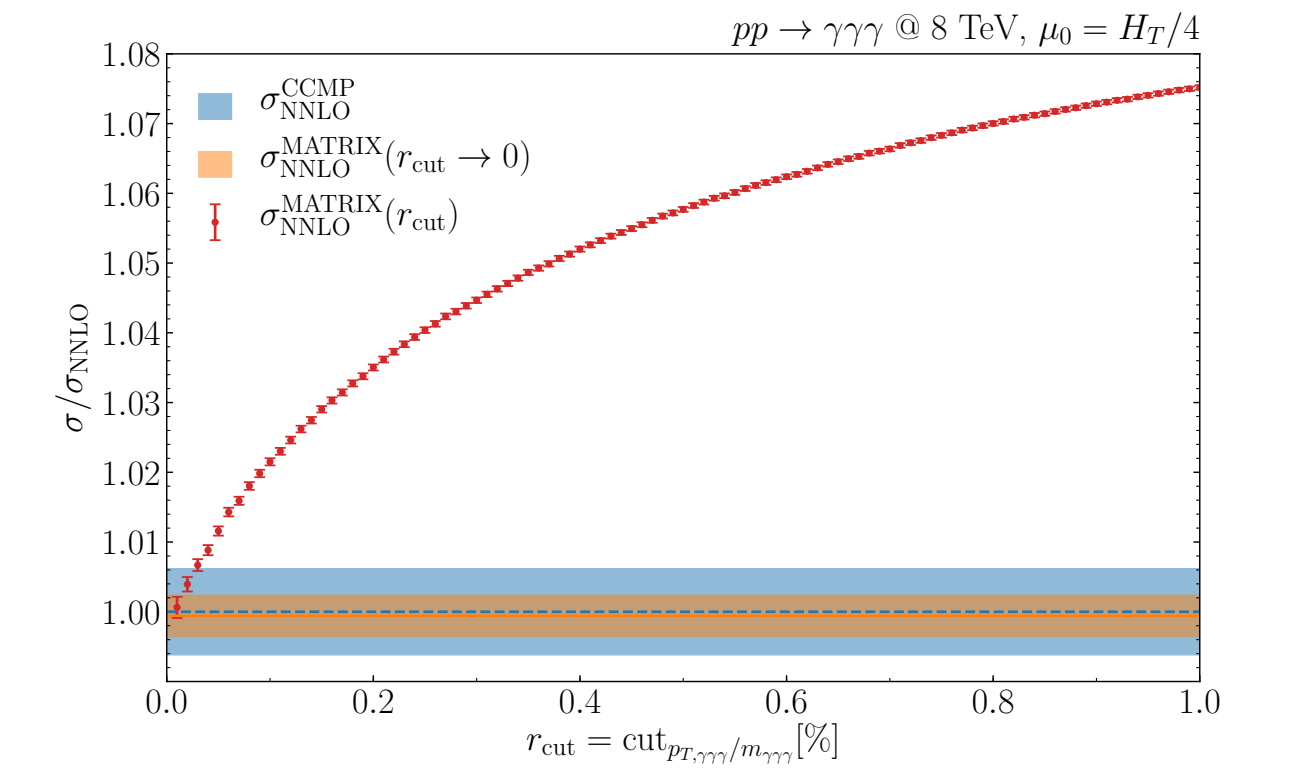
Uncertainties

- 7-point scale variation $0.5 \leq \mu_R/\mu_F \leq 2$
- r_{cut} extrapolation (small)
- PDF uncertainty 2-3% at NLO [arXiv:1712.07291] $\implies$ negligible at NNLO

$r_{\text{cut}} \to 0$ extrapolation

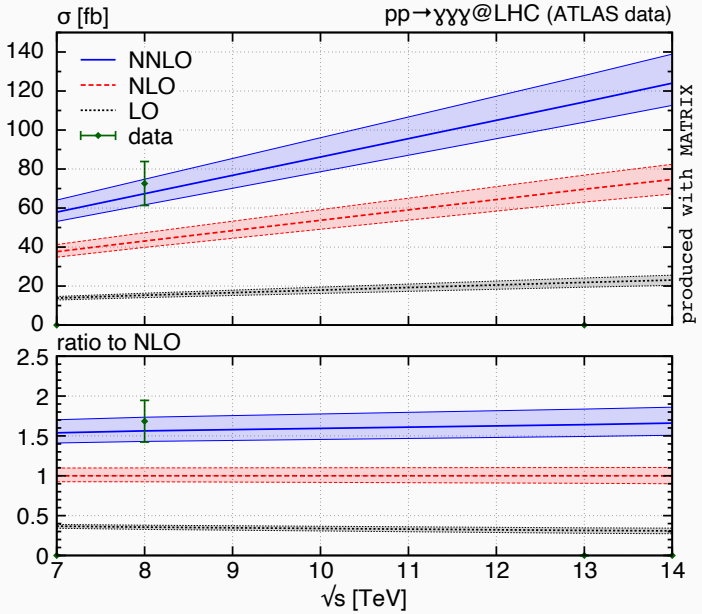
Three smooth-cone isolated photons, intricate interplay with r_{cut}

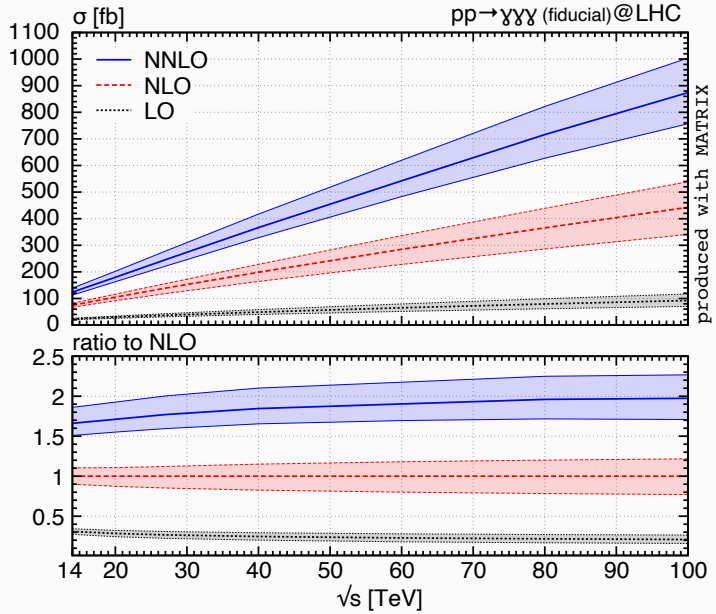
$\Longrightarrow$ potentially large uncertainties



- q_T subtraction fully capable dealing with $2 \to 3$ color singlet!
- extrapolation uncertainties controlled, few ‰, mild phase-space dependence

Fiducial cross sections

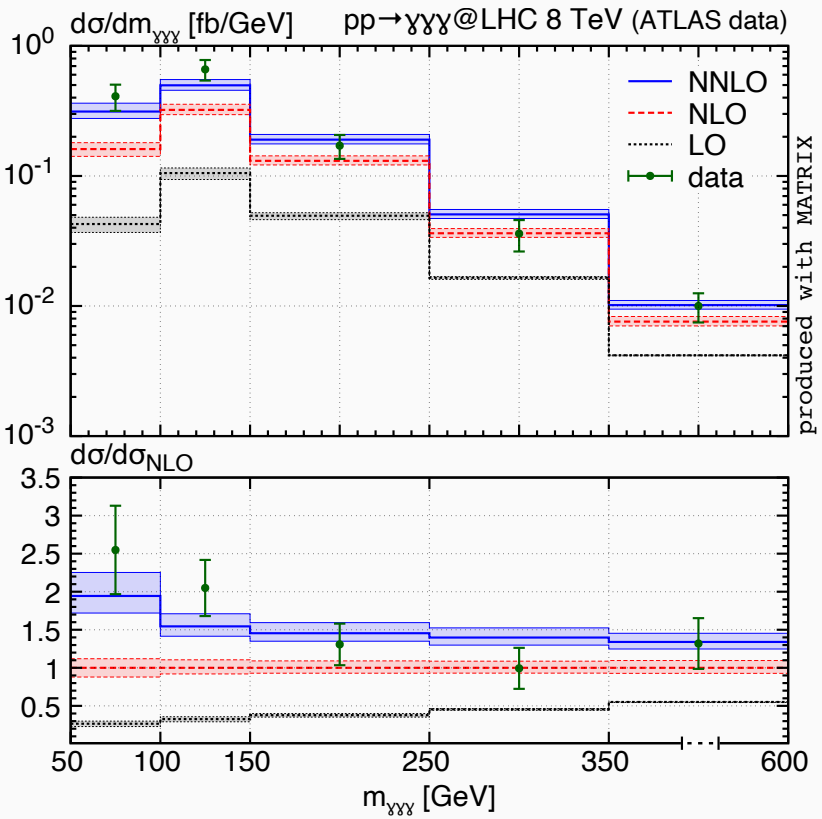


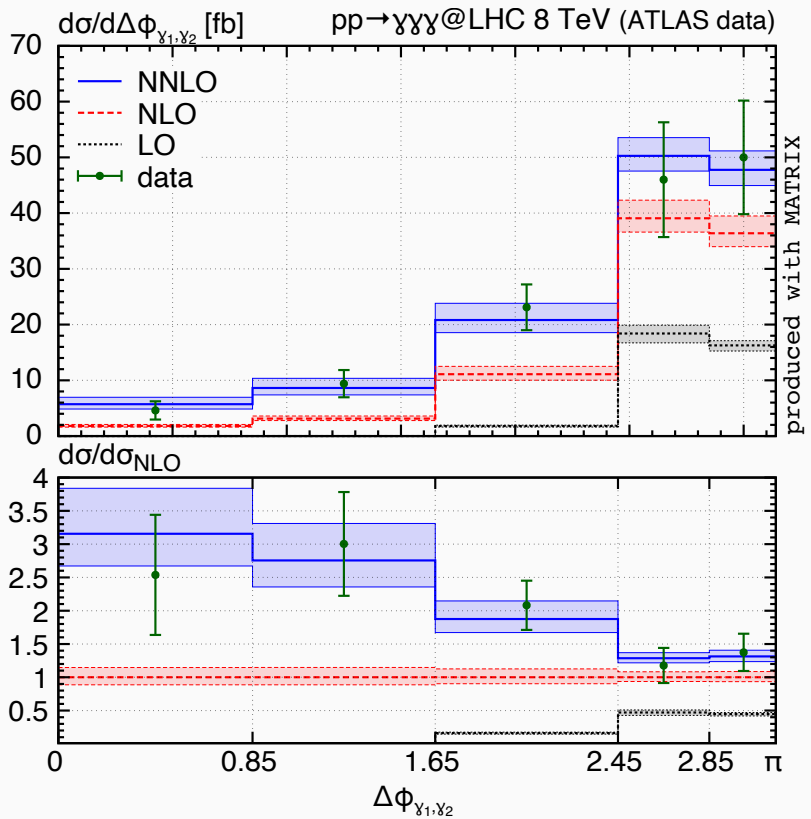


$\sqrt{s}$, TeV	σ_{NNLO}, fb	K_{NLO}	K_{NNLO}
7	$57.84(20)^{+10.7\%}_{-\ 8.3\%}$	2.72	1.54
8	$67.42(20)^{+11.0\%}_{-\ 8.5\%}$	2.82	1.56
13	$114.60(43)^{+11.9\%}_{-\ 9.1\%}$	3.18	1.65
14	$123.83(24)^{+12.0\%}_{-\ 9.2\%}$	3.24	1.66
27	$245.91(48)^{+13.2\%}_{-\ 9.9\%}$	3.76	1.77
100	$878.9(24)\ ^{+15.0\%}_{-13.5\%}$	4.79	1.99

- Full agreement with 8 TeV results of [Chawdry, Czakon, Mitov, Poncelet '19]
- Consistent with ATLAS 8 TeV measurement
  $72.6\ ^{+6.5}_{-6.5}(\mathrm{stat})\ ^{+9.2}_{-9.2}(\mathrm{syst})$ fb
- NNLO crucial for reliable prediction
- Gigantic K factors!

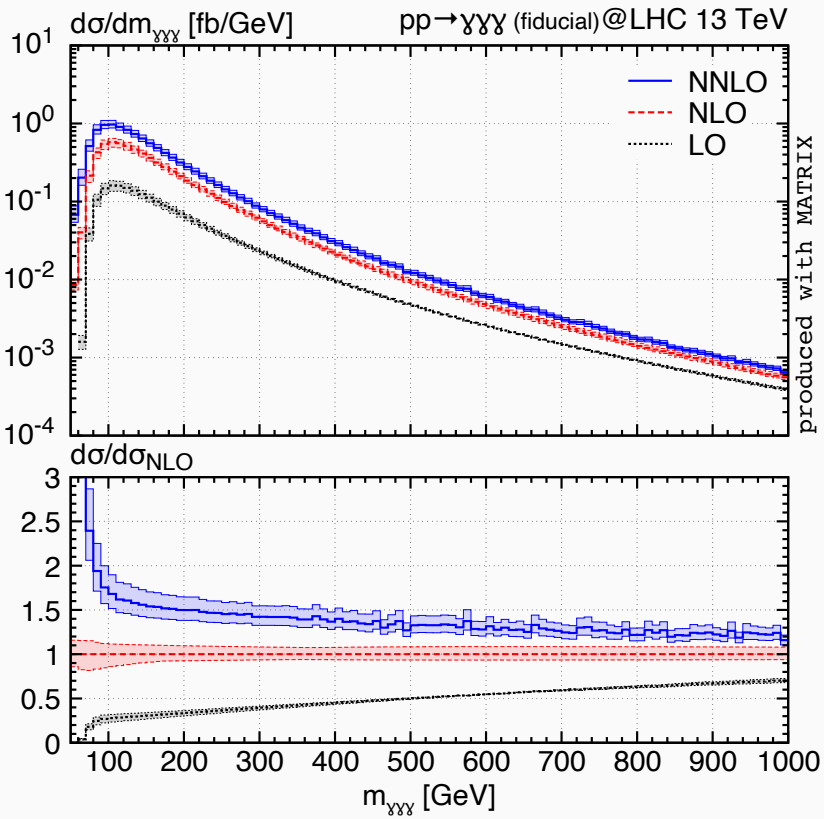
Differential cross sections $\sqrt{s} = 8$ TeV

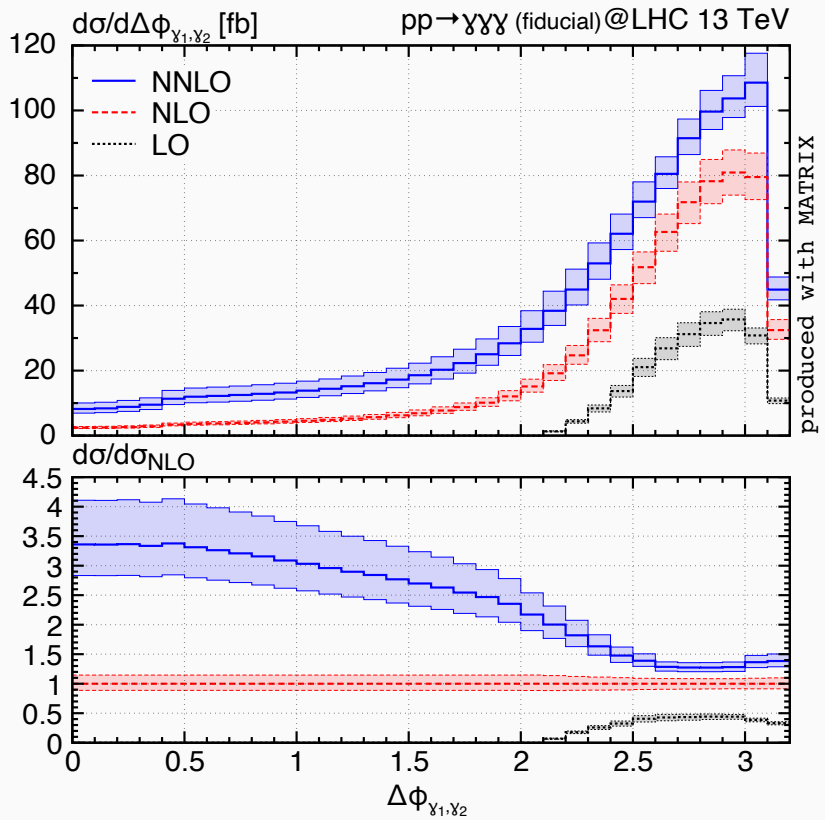




- Excellent agreement with data (and [Chawdry, Czakon, Mitov, Poncelet '19]) across all differential distributions
- Major shape differences

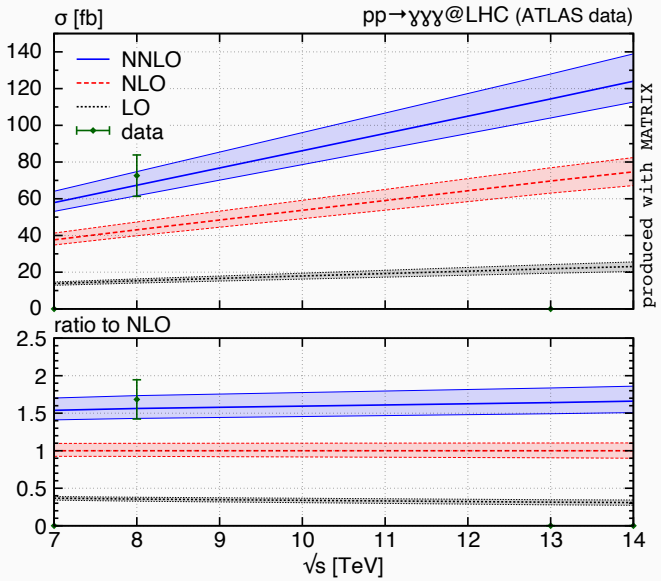
Differential cross sections $\sqrt{s} = 13$ TeV





- Similar pattern as in 8 TeV, corrections generally increase
- Efficient calculation allows fine binning, predictions for high-energy tails

Perturbative convergence



Symptoms

- Giant K_{NLO} and K_{NNLO} factors
- Uncertainty estimate from scale variations unreliable

Typical behavior

Lifting fixed-order constraints: opening partonic channels, degenerate kinematics.

Other examples: $\gamma\gamma$, $Wb\bar{b}$, H

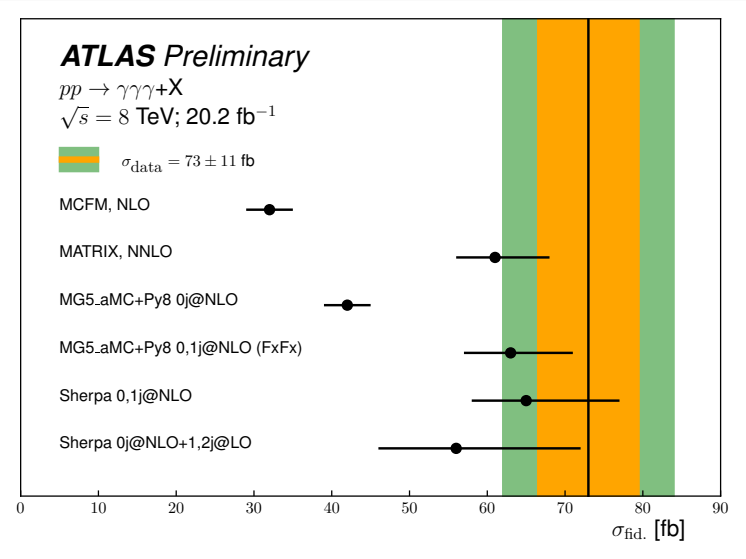
Extra: underestimated interplay of scale choice and isolation criteria?

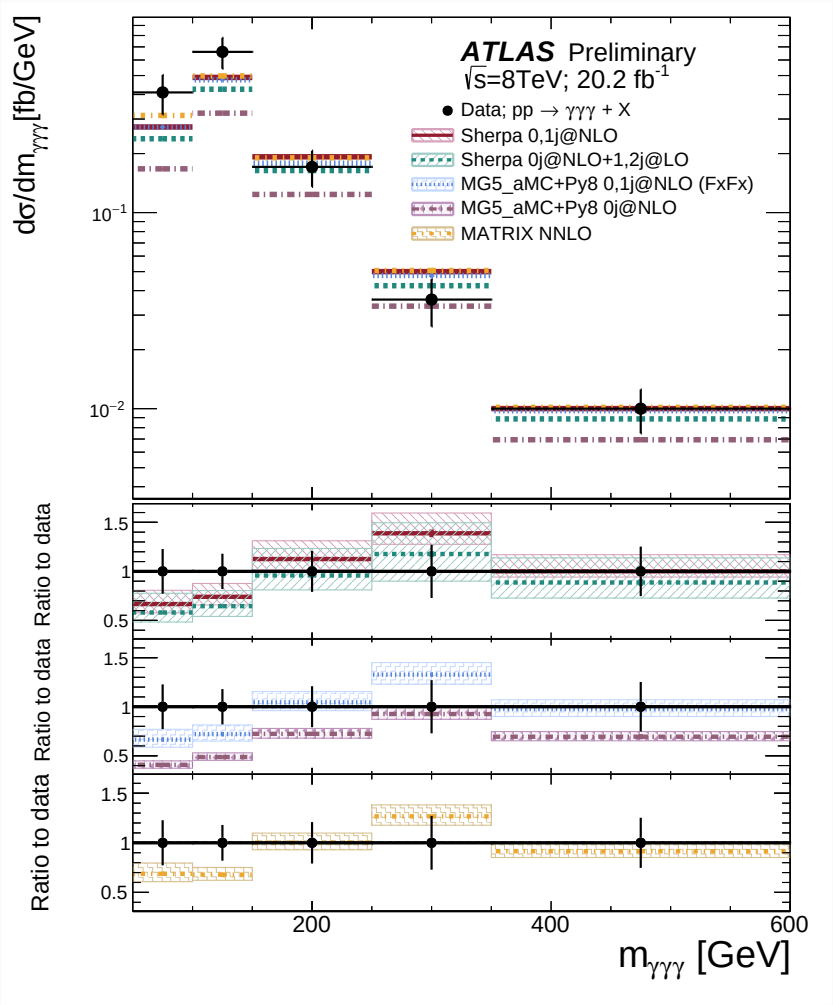
[Gehrmann, Glover, Huss, Whitehead '20]

For $pp \to \gamma\gamma\gamma + X$ first non-degenerate order is NNLO $\implies$ reliable uncertainties expected

Perturbative convergence

Comparison to merged 0,1j NLO sheds some light [ATL-PHYS-PUB-2021-001]





Conclusions & outlook

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- Pentagon functions: basis of transcendental functions for five-point massless scattering
  - Nice analytic structure $\Longrightarrow$ facilitates compact amplitudes.
  - Fast and stable public implementation `PentagonFunctions++`, tested in real applications.

- First pheno-ready analytic two-loop five-point amplitudes with Caravel.
  $pp \to \gamma\gamma\gamma$ and $pp \to 3\text{j}$ available in public `C++` library, seconds per phase-space point.

- Triphoton production in NNLO QCD with q_T-subtraction in Matrix
  - NNLO corrections large and essential to describe data.
  - First on-the-fly NNLO calculation of a $2 \to 3$ process.

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Outlook

- Will "pentagon functions" approach be the way to move forward beyond massless?
- Non-planar contributions: important, but two-loop amplitudes still difficult.
- Further improved predictions for triphoton production
  - Non-planar contributions, EW corrections, parton shower
  - Better understanding of uncertainties
- Three-jet amplitudes also available, looking forward for exciting phenomenology!