Recent advances in fixed-order calculations

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SM@LHC 2024, Rome, May 9, 2024

Recent highlights in fixed-order calculations

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The role of precision theory

After the discovery of the Higgs boson in 2012 no evidence of new phenomena has been reported yet

The LHC has accumulated only about 5-10% of the expected data, and surprises are still possible but it is difficult to expect a striking signal in the coming years

The most likely scenario is the one in which one or more consistent (small) deviations with respect the SM appear



The more accurate theory predictions are, the sooner can we be sensitive to these small deviations

Precision theory increases the discovery reach of the LHC and anticipates possible discoveries

Our starting point



High- p_T interactions are characterised by the presence of a hard scale Q(invariant mass of a lepton pair, high- p_T jet, heavy-quark mass...)



Can be controlled through the factorisation theorem

$$\sigma(P_1, P_2) = \sum_{i,j} \int dx_1 dx_2 f_{i/h_1}(x_1, \mu_F^2) f_{j/h_2}(x_2, \mu_F^2) \,\hat{\sigma}_{ij}(x_1 P_1, x_2 P_2, Q^2, \alpha_S(\mu_R); \mu_F^2, \mu_R^2) + \mathcal{O}\left[\left(\frac{\Lambda_{\text{QCD}}}{Q}\right)^F\right]$$

Parton distributions: universal but not perturbatively computable Hard partonic cross section: process dependent but computable in perturbation theory Power-suppressed contributions

 $\langle n \rangle$

1 .

The factorisation picture is systematically improvable (until the power-suppressed contributions become quantitative relevant...)

Fixed order predictions

Fixed order computations constitute the backbone of theory predictions at high-energy colliders

- Conceptually clean: systematic expansion in QCD and EW couplings (but technically more and more challenging as order increases)
- Compared to resummed computations, necessary when multiple scales are present, less prone to ambiguities
- Completely solved at NLO (both QCD and EW)

Openloops, Gosam, Madloop, NLOX, Recola....

• Still, difficult to assess theory uncertainties

see e.g. recent public discussion at https://indico.cern.ch/event/1368033

• Since $\alpha_S \gg \alpha$ the QCD effects are often (but not always !) the most important

How do we do these calculations ?

In short: we integrate matrix elements over phase space but...at each order we have more loops and more legs and

- amplitudes develop infrared (IR) singularities

- we need to be fully differential to adapt to realistic experimental cuts



Amplitudes:

At tree-level and one-loop they can be computed automatically

From two-loop on no general solution exists and complexity grows in **#loops** and **#scales**

Subtraction/slicing schemes:

Organise and cancel IR singularities

Efficiency becomes crucial as multiplicity increases

Cross validation between independent calculations essential

NNLO QCD progress



NNLO results lead to much better description of the data

$2 \rightarrow 2$: maturity

Benchmark 2 \rightarrow 2 processes VV, $Q\bar{Q}$ (Q = t, b), V+jet available since quite some time More recently:

● Flavoured jets: Z+b, Z+c, W+c → talk by Giovanni Stagnitto

Gauld et al (2020,2023) Czakon et al. (2023) Gehrmann et al (2023)

Behring et al (2020)

• Mass effects in H+jet and $gg \rightarrow ZZ$, ZH at NLO

Production and decay $pp \rightarrow WH(H \rightarrow b\bar{b})$

Kerner, Jones, Luisoni (2018) Del Duca et al (2023) Degrassi et al. (2021-24), Kerner et al (2022-24)....

Czakon et al (2021,2022)

Gehrmann et al (2022)

talk by Alessandro Vicini Bonciani, Buonocore, Vicini, MG (2021)

Buccioni et al (2022)

Inclusion of fragmentation

- identified hadrons
- photons 🔶 talk by Giovanni Stagnitto

Their impact can be of the same order as N³LO QCD effects

Mixed QCD-EW corrections

talk by Alessandro Vicini



Bonciani et al (2024)

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NNLO QCD progress



NNLO results lead to much better description of the data

$2 \rightarrow 3$: the frontier



$2 \rightarrow 3$: the frontier

Calculations of the two-loop virtual corrections with one or more masses typically performed in approximated form

Often in the leading-colour (LC) approximation $(N_c \gg 1)$

Other approximations exploit particular kinematical limits (e.g. soft or collinear approximations, small mass limits...)

One maybe obvious technical comment: whatever approximation is used, the singular terms have to be included exactly, in order to achieve a IR finite result

Quality of approximations may depend on the definition of the finite remainder Differences between LC and full color can be relatively large First exact $2 \rightarrow 3$ appeared for $pp \rightarrow \gamma jj$ (here subleading colour terms small) Badger et al (2023)

In general quality of approximations need to be checked case by case

ttH

Catani, Devoto, Kallweit, Mazzitelli, Savoini, MG (2022)

The associated production of the Higgs boson with a top-quark pair is a crucial process at the LHC

It allows a direct extraction of the top Yukawa



Experimental uncertainties are now at the O(20%)level but expected to go down to the 2% level at the end of the HL-LHC

Predictions based on NLO QCD+EW (+ resummations) affected by O(10%) uncertainty Missing ingredients for NNLO are the two-loop

 $gg \rightarrow t\bar{t}H$ and $q\bar{q} \rightarrow t\bar{t}H$ amplitudes

Recent progress:

- $q\bar{q} n_F$ part

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- one-loop at $\mathcal{O}(\epsilon^2)$
- some master integrals

- Heinrich et al (2024)
- Tancredi et al (2023)
 - Reina et al (2023)



ttH

The idea: use soft approximation for the missing two-loop amplitude

Tree-level soft-Higgs current

 $\mathcal{M}(\{p_i\},k) \simeq F(\alpha_S(\mu_R);m/\mu_R) J(k)\mathcal{M}(\{p_i\})$

Soft limit of the scalar heavy-quark form factor

Approximated term has very small impact

σ [pb]	$\sqrt{s} = 13 \mathrm{TeV}$	$\sqrt{s} = 100 \mathrm{TeV}$
$\sigma_{ m LO}$	$0.3910^{+31.3\%}_{-22.2\%}$	$25.38^{+21.1\%}_{-16.0\%}$
$\sigma_{ m NLO}$	$0.4875^{+5.6\%}_{-9.1\%}$	$36.43^{+9.4\%}_{-8.7\%}$
$\sigma_{ m NNLO}$	$0.5070(31)^{+0.9\%}_{-3.0\%}$	$37.20(25)^{+0.1\%}_{-2.2\%}$

NNLO effect is about +4% at 13 TeV and +2% at 100 TeV

Catani, Devoto, Mazzitelli, Kallweit, Savoini, MG (2022)

Bernreuther et al (2005); Blümlein et al (2017) Fael, Lange, Schönwald, Steinhauser (2022)



Buonocore, Devoto, Kallweit, Mazzitelli, Rottoli, Savoini, MG (2023)

Among the ttV signatures, ttW is special because it involves both EW and top sectors

It is at the same time a signal and a background to ttH and tttt and new physics searches

Since the top quark quickly decays into a W and a b jet, the signature is characterised by 3 W bosons

It provides an irreducible source of same-sign dilepton pairs relevant for many BSM searches

It is special compared to other $ttF(F = H, Z, \gamma)$ signatures because the W can only be emitted by the initial-state light quarks (no *gg* channel at LO)

ttW rate consistently higher than SM predictions

Here we use two different approximations of the missing two-loop amplitude

1) Use soft approximation for W emission with momentum k and polarisation $\varepsilon(k)$ to express ttW amplitude in terms of the $q\bar{q} \rightarrow t\bar{t}$ amplitude

$$\mathcal{M}(\{p_i\}, k, \mu_R; \epsilon) \simeq \frac{g}{\sqrt{2}} \left(\frac{p_2 \cdot \varepsilon(k)}{p_2 \cdot k} - \frac{p_1 \cdot \varepsilon(k)}{p_1 \cdot k} \right) \mathcal{M}_L(\{p_i\}, \mu_R; \epsilon)$$

$$\mathbf{f}_{\mathbf{q}_L \bar{q}_R \to t\bar{t} \text{ virtual amplitude}}$$

Bärnreuther et al. (2013) Mastrolia et al (2022)

2) Start from massless W+4 parton amplitudes

Abreu et al. (2021)

Use a "massification" procedure to obtain the leading terms in a $m_Q/Q \ll 1$ expansion

Penin (2006) Moch, Mitov (2007) Becher, Melnikov (2007)

Successfully applied to the NNLO computation of Wbb

Buonocore, Devoto, Kallweit, Mazzitelli, Rottoli, Savoini (2023)

Buonocore, Devoto, Kallweit, Mazzitelli,Rottoli, Savoini, MG (2023)

Both approximations provide a good estimate of the exact one-loop contribution

Soft approximation overshoots the exact results while massification tends to $p_{T,t|\tilde{t}^{7}}$ Trev overshoot it

Clear asymptotic behaviour towards exact result for high p_T of the top quarks where both approximations are expected to work

Buonocore, Devoto, Kallweit, Mazzitelli,Rottoli, Savoini, MG (2023)

The pattern is preserved at NNLO: massified result systematically higher than soft approximation

We define the uncertainty of each approximation as the maximum between what we obtain varying the subtraction scale $1/2 \le \mu_{\text{IR}}/Q \le 2$ and twice the NLO deviation

Our best prediction obtained as average of the two with linear combination of uncertainties

Final uncertainty on two-loop contribution about 25% and similar to what obtained in recent $2 \rightarrow 3$ calculations in leading color approximation

Abreu et al (2023)

Impact of two-loop virtual contribution: 6-7% of NNLO cross section

missing exact two-loop amplitudes

Large NLO QCD corrections (+50%)

Moderate NNLO corrections (+14-15%)

All subdominant LO and NLO contributions at $\mathcal{O}(\alpha^3)$, $\mathcal{O}(\alpha_S^2 \alpha^2)$, $\mathcal{O}(\alpha_S \alpha^3)$, $\mathcal{O}(\alpha^4)$ consistently included and denoted as NLO EW: effect is +5%

 $\sigma(t\bar{t}W^+)/\sigma(t\bar{t}W^-)$ only slightly decreases increasing the perturbative order

The comparison with the ATLAS and CMS results shows that discrepancy remains at the 1-20 level

Inclusion of NNLO corrections significantly reduces perturbative uncertainties

Our result is fully consistent with FxFx prediction but with smaller uncertainties

 $\sigma_{t\bar{t}W}^{\text{FxFx}} = 722.4^{+9.7\%}_{-10.8\%} \text{ fb}$

Similar situation with the new ATLAS measurement

Inclusion of NNLO corrections significantly reduces perturbative uncertainties

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 $\sigma_{t\bar{t}W}^{\text{FxFx}} = 722.4^{+9.7\%}_{-10.8\%} \text{ fb}$

N3LO: the frontier

For some benchmark processes NNLO may not be enough....

N3LO corrections for some 2->1 processes now available: total cross sections

		222 0				
	$Q \; [{ m GeV}]$	$\delta \sigma^{ m N^{o}LO}$	$\delta\sigma^{ m NNLO}$	$\delta(ext{scale})$	$\delta(\mathrm{PDF}+lpha_S)$	$\delta(ext{PDF-TH})$
$gg \rightarrow \text{Higgs}$	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%	$^{+0.66\%}_{-0.79\%}$	$+1.8\% \\ -1.9\%$	$\pm 2.5\%$
$\operatorname{CCDY}(W^+)$	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%	$^{+0.6\%}_{-0.5\%}$	$\pm 2\%$	$\pm 2.13\%$

Baglio et al (2022)

Small but significant impact of N3LO corrections, sometimes outside NNLO scale uncertainties

N3LO: the frontier

For some benchmark processes NNLO may not be enough....

N3LO corrections for some 2->1 processes now available: fully differential results

Projection to Born

Jet production in DIS

Higgs production in gluon fusion $H \rightarrow b\bar{b}$

 q_T subtraction

Higgs production in gluon fusion Drell-Yan Currie, Gehrmann, Glover, Huss Niehues (2018)

Gehrmann et al (2021)

Mondini, Schiavi, Williams (2019)

Cieri et al (2018) Gehrmann et al (2018)

Camarda, Cieri, Ferrera (2021-2023)

Gehrmann et al (2022), Campbell, Neumann (2022,23)

N3LO: the frontier

N3LO: PDFs

Current approximate N3LO fits use partial available information on N3LO splitting kernels

> Davies, Falcioni, Herzog, Moch, Ruijl, Soar Vermaseren, Vogt, Ueda....

Though approximate, this information should be sufficient to obtain sufficiently accurate PDFs evolution

Still large differences between the two existing aN3LO sets mainly in the charm and gluon density

These differences are most likely due to the different approaches and fitting methodologies

Summary & Outlook

- The lack of sufficiently precise theoretical predictions might lead to miss, or at least delay, possible discoveries
- NNLO results now available for essentially all the relevant 2->1 and $2 \rightarrow 2$ processes and lead to an improved description of the data
- Cross validation of different computations essential in consolidating the results but improvements in subtraction/slicing techniques expected/needed
- Extension to $2 \rightarrow 3$ requires facing new challenges in the computations of two-loop amplitudes: in the meanwhile approximations of the virtual allow us to achieve first NNLO accurate predictions
- NNLO computations challenging also from the point of view of computing resources

Only a limited subset of the results are publicly available

• N³LO era started with new exciting results and new challenges

Backup

ttH

When a soft photon (or gluon) is emitted in a high-energy process the corresponding amplitudes obey well known factorisation formulae

An analogous formula holds for the emission of a soft scalar off heavy quarks

 $\mathcal{M}(\{p_i\},k)\simeq J(k)\mathcal{M}(\{p_i\})$

At tree level it is straightforward to show that

$$J(k) = \sum_{i} \frac{m}{v} \frac{m}{p_i \cdot k}$$
heavy-quark momenta

Differences with other approaches

The idea of a treating the Higgs as a parton radiating off the top quark was used already in the past

Effective Higgs approximation in early NLO calculations: introduce a function expressing the probability to extract the Higgs boson from the top quark

Dawson and Reina (1997)

Fragmentation functions $D_{t \to H}$ and $D_{g \to H}$ evaluated at NLO

Brancaccio, Czakon, Gerenet, Krämer (2021)

These approaches are based on a collinear approximation

Our approximation is **purely soft** (collinear non-soft emissions are neglected but soft quantum interferences are included)

Moreover, we apply it only to the finite part of the two-loop contribution

The computation

We use the q_T subtraction method

Catani, MG (2007)

$$d\sigma_{NNLO}^{t\bar{t}H} = \mathscr{H}_{NNLO}^{t\bar{t}H} \otimes d\sigma_{LO}^{t\bar{t}H} + \left[d\sigma_{NLO}^{t\bar{t}H+\text{jets}} - d\sigma_{NNLO}^{CT} \right]$$

All the ingredients in this formula are now available and implemented in MATRIX except the two-loop virtual amplitudes entering \mathcal{H}

We define

$$\mathcal{H} = H\delta(1 - z_1)\delta(1 - z_2) + \delta\mathcal{H} \qquad \qquad H^{(n)} = \frac{2\text{Re}\left(\mathcal{M}_{\text{fin}}^{(n)}\mathcal{M}^{(0)*}\right)}{|\mathcal{M}^{(0)}|^2}$$

with

$$H = 1 + \frac{\alpha_{S}(\mu_{R})}{2\pi} H^{(1)} + \left(\frac{\alpha_{S}(\mu_{R})}{2\pi}\right)^{2} H^{(2)} + \dots \qquad \qquad |\mathcal{M}_{fin}(\mu_{IR})\rangle = \mathbb{Z}^{-1}(\mu_{IR}) |\mathcal{M}\rangle$$

IR subtraction

For n = 2 this definition allows us to single out the only missing ingredient in the NNLO calculation, that is, the coefficient $H^{(2)}$

Note that all the remaining terms are computed exactly (including $|\mathcal{M}_{fin}^{(1)}|^2$)

We have used our factorisation formula to construct approximations of the $H^{(1)}$ and $H^{(2)}$ coefficients

In order to use the factorisation formula we have to introduce a mapping that from a $t\bar{t}H$ event defines a $t\bar{t}$ event with no Higgs boson

To this purpose we use the q_T recoil prescription

Catani, Ferrera, de Florian, MG (2016)

With this prescription the momentum of the Higgs boson is equally reabsorbed by the initial state partons, leaving the top and antitop momenta unchanged

The required tree-level and one-loop amplitudes are obtained using **Openloops**

The $q\bar{q} \rightarrow t\bar{t}$ and $gg \rightarrow t\bar{t}$ two-loop amplitudes needed to apply our approximation are those provided by Czakon et al.

Bärnreuther, Czakon, Fiedler (2013)

Setup: NNPDF31 NNLO partons with 3-loop α_S $m_H = 125 \text{ GeV}$ and $m_t = 173.3 \text{ GeV}$

> Central values for factorisation and renormalisation scales $\mu_F = \mu_R = (2m_t + m_H)/2$ 33

Our first check is on the LO cross sections: we find that the soft approximation overestimates it by

- gg channel: a factor of 2.3 at $\sqrt{s} = 13$ TeV and a factor of 2 at $\sqrt{s} = 100$ TeV
- $q\bar{q}$ channel: a factor of 1.11 at $\sqrt{s} = 13$ TeV and a factor of 1.06 at $\sqrt{s} = 100$ TeV

These are absolute LO predictions: in our calculation we will actually need to approximate $H^{(1)}$ and $H^{(2)}$ that are normalised to LO matrix elements

$$H^{(n)} = \frac{2\operatorname{Re}\left(\mathscr{M}_{\operatorname{fin}}^{(n)}\mathscr{M}^{(0)*}\right)}{\left|\mathscr{M}^{(0)}\right|^2}$$

We expect this approximation to work better than simply computing $2\text{Re}\left(\mathcal{M}_{\text{fin}}^{(n)}\mathcal{M}^{(0)*}\right)$: effective reweighing of LO cross section

When computing virtual amplitudes we will set the infrared subtraction scale μ_{IR} to the invariant mass of the final state system

	$\sqrt{s} = 13 \mathrm{TeV}$		$\sqrt{s} = 100 \mathrm{TeV}$	
$\sigma~\mathrm{[fb]}$	gg	qar q	gg	q ar q
$\sigma_{ m LO}$	261.58	129.47	23055	2323.7
$\Delta\sigma_{ m NLO,H}$	88.62	7.826	8205	217.0
$\Delta \sigma_{ m NLO,H} _{ m soft}$	61.98	7.413	5612	206.0

We now move to NLO and compare the exact contribution from $H^{(1)}$ to the one computed in the soft approximation

The hard contribution computed in the soft approximation is underestimated by just 30 % in the *gg* channel and by 5 % in the $q\bar{q}$

The mismatch that we observe at NLO can be used to estimate the uncertainty of our approximation at NNLO

The quality of our final result will depend on the size of the contribution we approximate

	$\sqrt{s} = 13 \mathrm{TeV}$		$\sqrt{s} = 100 \mathrm{TeV}$	
$\sigma~[{ m fb}]$	gg	qar q	gg	qar q
$\sigma_{ m LO}$	261.58	129.47	23055	2323.7
$\Delta\sigma_{ m NLO,H}$	88.62	7.826	8205	217.0
$\Delta\sigma_{ m NLO,H} _{ m soft}$	61.98	7.413	5612	206.0
$\Delta \sigma_{ m NNLO,H} _{ m soft}$	-2.980(3)	2.622(0)	-239.4(4)	65.45(1)

At NNLO the hard contribution is about 1% of the LO cross section in the gg channel and 2% in the $q\bar{q}$ channel

We can therefore anticipate that at NNLO the uncertainties due to the soft approximation will be rather small.

But how can we estimate these uncertainties ?

We have carefully studied the stability of our results under variations of the approximation procedure

• We have varied the recoil procedure: reabsorbing the Higgs momentum in just one of the initial state partons leads to negligible differences

We have repeated our computation by using different subtraction scales at which the finite part of the two-loop virtual amplitude in $H^{(2)}$ is defined

When varying μ_{IR} from *M*/2 to 2*M* and adding the exact evolution terms from these scales back to *M*

- In the gg channel we find $^{+164\%}_{-25\%}$ at 13 TeV and $^{+142\%}_{-20\%}$ at 100 TeV
- In the $q\bar{q}$ channel we find $^{+4\%}_{-0\%}$ at 13 TeV and $^{+3\%}_{-0\%}$ at 100 TeV

To define our uncertainties we start from the NLO result: the hard contribution computed in the soft approximation is underestimated by just 30% in the gg channel and by 5% in the $q\bar{q}$ therefore the NNLO uncertainty cannot be smaller than these values

We multiply these uncertainties by a tolerance factor of 3 We finally combine the *gg* and $q\bar{q}$ uncertainties linearly $\implies \pm 0.6\%$ on σ_{NNLO}

Results

σ [pb]	$\sqrt{s} = 13 \mathrm{TeV}$	$\sqrt{s} = 100 \mathrm{TeV}$
$\sigma_{ m LO}$	$0.3910^{+31.3\%}_{-22.2\%}$	$25.38^{+21.1\%}_{-16.0\%}$
$\sigma_{ m NLO}$	$0.4875^{+5.6\%}_{-9.1\%}$	$36.43^{+9.4\%}_{-8.7\%}$
$\sigma_{ m NNLO}$	$0.5070(31)^{+0.9\%}_{-3.0\%}$	$37.20(25)^{+0.1\%}_{-2.2\%}$

NLO effect is about +25% at 13 TeV and +44% at 100 TeV

NNLO effect is about +4% at 13 TeV and +2% at 100 TeV

Significant reduction of perturbative uncertainties

Errors in bracket obtained combining uncertainty from the soft approximation and the q_T subtraction systematics (same procedure used in MATRIX)

Higgs p_T spectrum

Uncertainties from soft-approximation over the Higgs p_T spectrum remain of the same order (a similar uncertainty is obtained by using μ_{IR} variations)

At first sight this is counterintuitive since at large $p_{T,H}$ the soft approximation is expected to become worse !

However at large $p_{T,H}$ the role of the *gg* channel is reduced and the $q\bar{q}$ channel, which is under better control, plays the major role

As done for $t\bar{t}H$ we have used our factorisation formulas to construct approximations of the $H^{(1)}$ and $H^{(2)}$ coefficients

To properly define our approximations we need momentum mappings

- For the soft-W approximation we absorb the W momentum into the top quarks, thus preserving the invariant mass of the event

- For the massification we map the momenta of the massive top quarks into massless momenta by preserving the four-momentum of the pair

Required tree-level and one-loop amplitudes obtained using Openloops and Recola

- The $q\bar{q} \rightarrow t\bar{t}$ two-loop amplitudes needed to apply our soft approximation are those provided by Czakon et al. Bärnreuther, Czakon, Fiedler (2013); Mastrolia et al (2022)

- The W+4 parton massless two-loop amplitudes needed to use massification are those from Abreu et al (leading colour approximation) Abreu et al (2021)

Setup: NNPDF31_nnlo_as_0118_luxqed partons with 3-loop α_S $\sqrt{s} = 13 \text{ TeV}$ Central values for factorisation and renormalisation scales $\mu_F = \mu_R = (2m_t + m_W)/2 \equiv = M/2$

Perturbative uncertainties

Our predictions are obtained by using $\mu_0 = M/2$ as central scale and performing standard 7-point scale variations

We have repeated our calculation using $H_T/2$, $H_T/4$ and M/4 as central scales

The four predictions are fully consistent within their uncertainties

Symmetrising the *M*/2 scale uncertainty we obtain an upper bound that is almost identical to that of $\mu_0 = M/4$ and $\mu_0 = H_T/4$

We find that the NNLO correction is dominated by virtual and real contributions in the qg channel: no new large contribution from channels opening up at NNLO (as gg)

We take the $\mu_0 = M/2$ as reference and use symmetrised scale variations as estimate of our uncertainties