Scalable NNLO Phenomenology

Radja Boughezal

Argonne National Laboratory

ACAT 2016, Valparaiso, January 18-22
• Recent breakthrough in High Energy Particle Physics: a Higgs was discovered in 2012!

Is this the predicted Standard Model Higgs? Could there be hidden new physics? Can only tell if SM signal and backgrounds are predicted very precisely.

• From the U.S. DOE: “...The full discovery potential of the Higgs will be unleashed by percent-level precision studies of the Higgs properties. The measurement of these properties is a top priority in the physics program of high-energy colliders.”

Particle Physics Project Prioritization Panel (P5) report
• Recent breakthrough in High Energy Particle Physics: a Higgs was discovered in 2012!

Is this the predicted Standard Model Higgs? Could there be hidden new physics? Can only tell if SM signal and backgrounds are predicted very precisely. Goal can be achieved if we have:

Sophisticated box of tools

Automatic packages for cross section calculations

New techniques for calculating high precision predictions

Radja Boughezal, ANL

Scalable NNLO Phenomenology
LHC Run 1 & Theory

### ATLAS

<table>
<thead>
<tr>
<th>Source of uncertainty</th>
<th>$4\mu$</th>
<th>$2e2\mu$</th>
<th>$2\mu2e$</th>
<th>$4e$</th>
<th>combined</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electron reconstruction and identification efficiencies</td>
<td>–</td>
<td>1.7%</td>
<td>3.3%</td>
<td>4.4%</td>
<td>1.6%</td>
</tr>
<tr>
<td>Electron isolation and impact parameter selection</td>
<td>–</td>
<td>0.07%</td>
<td>1.1%</td>
<td>1.2%</td>
<td>0.5%</td>
</tr>
<tr>
<td>Electron trigger efficiency</td>
<td>–</td>
<td>0.21%</td>
<td>0.05%</td>
<td>0.21%</td>
<td>&lt;0.2%</td>
</tr>
<tr>
<td>$\ell\ell + ee$ backgrounds</td>
<td>–</td>
<td>–</td>
<td>3.4%</td>
<td>3.4%</td>
<td>1.3%</td>
</tr>
<tr>
<td>Muon reconstruction and identification efficiencies</td>
<td>1.9%</td>
<td>1.1%</td>
<td>0.8%</td>
<td>–</td>
<td>1.5%</td>
</tr>
<tr>
<td>Muon trigger efficiency</td>
<td>0.6%</td>
<td>0.03%</td>
<td>0.6%</td>
<td>–</td>
<td>0.2%</td>
</tr>
<tr>
<td>$\ell\ell + \mu\mu$ backgrounds</td>
<td>1.6%</td>
<td>1.6%</td>
<td>–</td>
<td>–</td>
<td>1.2%</td>
</tr>
</tbody>
</table>

- **QCD scale uncertainty**: 6.5%
- **PDF, $\alpha_s$ uncertainty**: 6.0%
- **$H \rightarrow ZZ^*$ branching ratio uncertainty**: 4.0%
## LHC Run 1 & Theory

### ATLAS

#### H → WW*

**Observed μ = 1.09**

<table>
<thead>
<tr>
<th>Source</th>
<th>Error</th>
<th>Plot of error (scaled by 100)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Data statistics</strong></td>
<td>0.16 0.15</td>
<td></td>
</tr>
<tr>
<td>Signal regions</td>
<td>0.12 0.12</td>
<td></td>
</tr>
<tr>
<td>Profiled control regions</td>
<td>0.10 0.10</td>
<td></td>
</tr>
<tr>
<td>Profiled signal regions</td>
<td>- -</td>
<td></td>
</tr>
<tr>
<td><strong>MC statistics</strong></td>
<td>0.04 0.04</td>
<td></td>
</tr>
<tr>
<td>Theoretical systematics</td>
<td>0.15 0.12</td>
<td></td>
</tr>
<tr>
<td>Signal $H \rightarrow WW^*$ B</td>
<td>0.05 0.04</td>
<td></td>
</tr>
<tr>
<td>Signal ggF cross section</td>
<td>0.09 0.07</td>
<td></td>
</tr>
<tr>
<td>Signal ggF acceptance</td>
<td>0.05 0.04</td>
<td></td>
</tr>
<tr>
<td>Signal VBF cross section</td>
<td>0.01 0.01</td>
<td></td>
</tr>
<tr>
<td>Signal VBF acceptance</td>
<td>0.02 0.01</td>
<td></td>
</tr>
<tr>
<td>Background $WW$</td>
<td>0.06 0.06</td>
<td></td>
</tr>
<tr>
<td>Background top quark</td>
<td>0.03 0.03</td>
<td></td>
</tr>
<tr>
<td>Background misid. factor</td>
<td>0.05 0.05</td>
<td></td>
</tr>
<tr>
<td>Others</td>
<td>0.02 0.02</td>
<td></td>
</tr>
<tr>
<td><strong>Experimental systematics</strong></td>
<td>0.07 0.06</td>
<td></td>
</tr>
<tr>
<td>Background misid. factor</td>
<td>0.03 0.03</td>
<td></td>
</tr>
<tr>
<td>Bkg. $Z/\gamma^* \rightarrow ee, \mu\mu$</td>
<td>0.02 0.02</td>
<td></td>
</tr>
<tr>
<td>Muons and electrons</td>
<td>0.04 0.04</td>
<td></td>
</tr>
<tr>
<td>Missing transv. momentum</td>
<td>0.02 0.02</td>
<td></td>
</tr>
<tr>
<td>Jets</td>
<td>0.03 0.02</td>
<td></td>
</tr>
<tr>
<td>Others</td>
<td>0.03 0.02</td>
<td></td>
</tr>
<tr>
<td><strong>Integrated luminosity</strong></td>
<td>0.03 0.03</td>
<td></td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>0.23 0.21</td>
<td></td>
</tr>
</tbody>
</table>

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Scalable NNLO Phenomenology
**LHC Run 1 & Theory**

**ATLAS**

<table>
<thead>
<tr>
<th>Source of uncertainty</th>
<th>( H \rightarrow WW^* )</th>
<th>( H \rightarrow ZZ^* )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electron reconstruction and isolation and impurities</td>
<td>Source</td>
<td>Error</td>
</tr>
<tr>
<td></td>
<td></td>
<td>+</td>
</tr>
<tr>
<td>Muon reconstruction and isolation and impurities</td>
<td>Muon trigger efficiency</td>
<td>2.5%</td>
</tr>
<tr>
<td>Muon trigger efficiency</td>
<td>Muon trigger efficiency</td>
<td>2.5%</td>
</tr>
<tr>
<td>QCD scale factor</td>
<td>QCD scale factor</td>
<td>1.0%</td>
</tr>
<tr>
<td>PDF, ( \alpha_s ) uncernty</td>
<td>PDF, ( \alpha_s ) uncernty</td>
<td>0.5%</td>
</tr>
</tbody>
</table>

**Uncertainty group**

<table>
<thead>
<tr>
<th>Source</th>
<th>( \sigma_{\text{syst}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theory (yield)</td>
<td>0.09</td>
</tr>
<tr>
<td>Experimental (yield)</td>
<td>0.02</td>
</tr>
<tr>
<td>Luminosity</td>
<td>0.03</td>
</tr>
<tr>
<td>MC statistics</td>
<td>(&lt; 0.01 )</td>
</tr>
<tr>
<td>Theory (migrations)</td>
<td>0.03</td>
</tr>
<tr>
<td>Experimental (migrations)</td>
<td>0.02</td>
</tr>
<tr>
<td>Resolution</td>
<td>0.07</td>
</tr>
<tr>
<td>Mass scale</td>
<td>0.02</td>
</tr>
<tr>
<td>Background shape</td>
<td>0.02</td>
</tr>
</tbody>
</table>
For all three Higgs ‘precision’ channels, theory uncertainty is the dominant source of systematic uncertainty!
Easter morning excitement as the CERN accelerator team send beams around the LHC for the first time in many months - a major milestone on the way to even higher energy collisions!

(05–Apr–2015 10:40:17)
All collimators open Circulating beam 2

Big Bang Beam: Large Hadron Collider Restarts After Two-Year Break

LHC restart: 'We want to break physics'

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LHC Run 2: Prospects

- High expectations from the higher energy (13-14 TeV) and luminosity (~300fb⁻¹)

Scenario 1: all systematic uncertainties same as now
Scenario 2: scale theory unc. by 1/2, experimental sys. by 1/sqrt(L)

Large impact from theory uncertainties (dashed) coming from QCD scale, jet binning, PDF+\(\alpha_s\)
How we make predictions for the LHC

- For low multiplicity processes include higher order terms in the fixed order calculations (LO $\rightarrow$ NLO $\rightarrow$ NNLO,...)

$$\Rightarrow \quad \sigma = \sigma_0 + \alpha_s \sigma_1 + \alpha_s^2 \sigma_2 + \ldots$$

- For higher multiplicity use the tree-level results when NLO is not available
How we make predictions for the LHC

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![Graph showing number of loops and additional legs](image)

First reliable predictions error ~ 10-30%
How we make predictions for the LHC

- For low multiplicity processes include higher order terms in the fixed order calculations (LO $\to$ NLO $\to$ NNLO, ...)

$$\Rightarrow \sigma = \sigma_0 + \alpha_s \sigma_1 + \alpha_s^2 \sigma_2 + \ldots$$

- For higher multiplicity use the tree-level results when NLO is not available

First precision predictions error $\sim$ few %
NNLO Cross Sections
The Importance of Higher Orders

• Example: until recently, \( WW \) cross section showed a >2\( \sigma \) excess at both ATLAS and CMS, and for both 7 and 8 TeV. Could it be light charginos? (Curtin, Jaiswal, Meade 1206.6888)

• Sizable NNLO QCD corrections!
  Gehrmann, Grazzini, Kallweit, Maierhofer, von Manteuffel, Pozzorini, Rathlev, Tancredi 1408.5243

• Additional enhancement when extrapolating from 0-jet bin to full cross section
  Curtin, Meade, Tien 1406.0848; Jaiswal, Okui, 1407.4537; Monni, Zanderighi 1410.4745

• Theory within 1\( \sigma \) agreement of ATLAS and CMS for both CM energies; proper interpretation not possible without NNLO QCD
Ingredients for NNLO Calculations

- Need the following ingredients for NNLO cross sections

IR singularities cancel in the sum of real and virtual corrections and mass factorization counterterms but only after phase space integration for real radiations.

- Virtual corrections have explicit IR poles, whereas real corrections have implicit IR poles that need to be extracted.

- A generic procedure to extract IR singularities from RR and RV was unknown when jets in the final state are involved, until very recently.
A Time Line for NNLO Hadron Collider Cross Sections

- Complete NNLO hadron-collider cross sections with control over kinematics:

- NNLO has become the standard for 2→2 scattering over the past 2-3 years
Techniques for NNLO

• Numerous proposed techniques for handling singularities at NNLO, which can be divided into two distinct categories:

**(quasi-)Local:** add and subtract counterterms that approximate real-emission matrix elements in all singular limits

**Resummation-assisted:** leverage knowledge of analytic resummation to remove double-real emission singularities.

**Local:**

• *Sector decomposition:* Binoth, Heinrich; Anastasiou, Melnikov, Petriello
• *Antennae subtraction:* Gehrmann, Gehrmann-de Ridder, Glover
• *Sector-improved residue subtraction:* Czakon; RB, Melnikov, Petriello
• *Colorful subtraction:* Del Duca, Somogyi, Trocsanyi
• *Projection-to-Born:* Cacciari, Dreyer, Karlberg, Salam, Zanderighi

**RG-assisted:**

• *q_T-subtraction:* Catani, Grazzini
• *N-jettiness subtraction:* RB, Focke, Liu, Petriello; Gaunt, Stahlhofen, Tackmann, Walsh
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RG-assisted:

• $q_T$-subtraction: Catani, Grazzini
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Numerous proposed techniques for handling singularities at NNLO, which can be divided into two distinct categories:

- **(quasi-)Local**: add and subtract counterterms that approximate real-emission matrix elements in all singular limits.
- **Resummation-assisted**: leverage knowledge of analytic resummation to remove double-real emission singularities.
For color-neutral final states, the transverse momentum completely determines the double-unresolved singular limit of the final state \cite{Catani:2007vq}.

\[
\sigma_{NNLO} = \int dq_T \frac{d\sigma}{dq_T} \theta(q_T^{cut} - q_T) + \int dq_T \frac{d\sigma}{dq_T} \theta(q_T - q_T^{cut})
\]

Obtained from the Collins-Soper-Sterman factorization theorem for small-\(q_T\).

Maximally reuses information from existing NLO calculations.

Computationally efficient.
**q_T-subtraction**

- Difficult to extend beyond color-neutral final states; $q_T$ no longer separates double-unresolved limit from NLO singular limits

Need a different resolution parameter when final-state jets are present!

- Two requirements: must separate double-unresolved limits from single-unresolved and hard regions, and must be resummable
N-jettiness

- N-jettiness, $\tau_N$: a resummable event-shape variable designed to veto final-state jets. Stewart, Tackmann, Waalewijn 0910.0467

$$\tau_N = \sum_k \min_i \left\{ \frac{2p_i \cdot q_k}{Q_i} \right\}.$$ 

- $N =$ number of final-state jets
- Momenta of the two beams and the final-state jets
- All final-state partons
- Measure of the jet hardness (we take $Q_i = 2E_i$)

$\tau_N = 0$: all radiation is either soft, or collinear to a beam/jet; at NNLO, gives the double-unresolved limit

$\tau_N > 0$: at least one additional radiation is resolved; have $N+1$ final-state jets

This is the resolution parameter we are looking for!
N-jettiness

- N-jettiness can be applied to obtain exact NNLO cross sections

$\tau_N \approx 0$: all radiation is either soft, or collinear to a beam/jet; at NNLO, gives the double-unresolved limit

$\tau_N > 0$: at least one additional radiation is resolved; have N+1 final-state jets

$$\tau_N = \sum \min_i \left\{ \frac{2p_i \cdot q_k}{Q_i} \right\}$$

Must all nearly vanish for $\tau_N \approx 0$

Must have at least one dot product non-vanishing; clearly can obtain from an NLO calculation with N+1 jets
W+jet$@_{NNLO}$

- W+jet and the associated W-$p_T$ spectrum are important benchmark processes in the SM.
- Can be used to determine the high-x gluon PDF, at ATLAS/CMS or LHCb. In the latter case, the NLO theoretical error is a limiting factor [Farry, Gauld 1505.01399].
W+jet@NNLO: validation

- A powerful check of the N-jettiness subtraction formalism is the independence of the final result from $\tau_N^{cut}$.

- The above-cut and below cut contributions separately depend on $\ln^n(\tau_N^{cut})$, where $n$ ranges from 1 to 4 at NNLO. This dependence must cancel when the two regions are summed.

- CMS cuts: $p_{TJ}>30$ GeV, $|\eta_J|<2.4$

- CT10 PDFs, $\mu_0=M_W$, vary by factor of 2 to estimate error

- NLO prediction using N-jettiness agrees with known results.

- Sum of above-cut and below-cut contributions stable to better than 0.1% of $\sigma_{total}$
• Tiny NNLO corrections; at the -1% level for the central scale choice ($\mu = m_W$)

• For transverse momenta less than 200 GeV, ratio of NNLO over NLO cross section is flat (with the exception of the Sudakov shoulder in the $p_{TW}$ distribution caused by the $p_{TJ}>30$ GeV cut)
Tiny NNLO corrections; at the -1% level for the central scale choice.

For transverse momenta less than 200 GeV, ratio of NNLO over NLO cross section is flat (with the exception of the Sudakov shoulder in the $p_TW$ distribution caused by the $p_{TJ}>30$ GeV cut)

All numerical results obtained in ~few hours using R.B., Focke, Liu, Petriello 1504.02131
**H+jet@NNLO: validation**

- An additional check is possible in this case. The dominant $qg$ and $gg$ scattering channels were also computed using the sector-improved residue subtraction technique. 

  R.B., Caola, Melnikov, Petriello, Schulze 1504.07922

- Agreement between the two calculations at the permille level

- Effect of missing $qq$ channels in the sector-improved calculation at the 1-2% level

- Reduced scale dependence at NNLO; preference for smaller scales

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**Important, unique validation of NNLO calculational technology!**
H+jet@NNLO: validation

- An additional check is possible in this case. The dominant qg and gg scattering channels were also computed using the sector-improved residue subtraction technique.

- Good perturbative behavior and smaller uncertainties for all differential distributions ($p_{TH}$, $p_{Tj}$, $Y_j$).

- Corrections in inclusive $\sigma$ are 20% for $\mu = m_H$ and 4% for $\mu = m_H/2$.

- Agreement between the two calculations at the permille level.

- Effect of missing qq channels in the sector-improved calculation at the 1-2% level.

- Reduced scale dependence at NNLO; preference for smaller scales.

Important, unique validation of NNLO calculational technology!
• NNLO corrections are flat as a function of jet rapidity
• However, the NNLO/NLO ratio for the $p_{TJ}$ distribution varies by ~20% as $p_{TJ}$ is varied from 30 GeV to 180 GeV (similar observation for $p_{TH}$)
**Z+jet@NNLO**

- **Z+jet** is another important SM benchmark; needed for gluon PDF determination; detector calibration; background to dark matter searches in the mono-jet channel

\[
\mu = \sqrt{M_{ll}^2 + \sum_j p_{T,j}^2}
\]

- Z-boson $p_T$ and $Y$ receive small NNLO corrections, with a flat $K$-factor

---

**Figure**

- Graphs showing the distribution of $d\sigma/dp_T^Z$ and $d\sigma/dY^Z$ at 13 TeV for LO, NLO, and NNLO calculations.

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**References**

R.B., Campbell, Ellis, Focke, Giele, Liu, Petriello 1512.01291
Z+jet@NNLO

- Z+jet is another important SM benchmark; needed for gluon PDF determination; detector calibration; background to dark matter searches in the mono-jet channel.

- NNLO jet distribution corrections also small, even though NLO corrections are large and very dependent on kinematics.
• **Z+jet** is another important SM benchmark; needed for gluon PDF determination; detector calibration; background to dark matter searches in the mono-jet channel

- **Z+jet ready for precision studies at the LHC Run II**

- **NNLO jet distribution corrections also small, even though NLO corrections are large and very dependent on kinematics**
Public Release of the NNLO Code

- A nice feature of N-jettiness subtraction is that it maximally reuses information available in existing NLO calculations/codes.
- This simplifies the public release of NNLO results: we can build upon existing NLO codes.
- We have calculated W+j, Z+j, H+j, as well as inclusive W/Z/H cross sections @ NNLO and incorporated them within the MCFM framework. We can do the same with any other NLO results/codes.
THE ERA OF SUPERCOMPUTERS

National Energy Research Scientific Computing Center, Berkeley

Edison System Configuration
- Architecture: Cray XC3
- Nodes: 5,576
- Cores/node: 24
- Total cores: 133,824 cores
- Memory/node: 64 GB RAM per node
- Memory/core: 2.66 GB

Mira System Configuration
- Architecture: IBM BG/Q
- Nodes: 49,152
- Cores/node: 16
- Total cores: 786,432 cores
- Memory/node: 16 GB RAM per node
- Memory/core: 1 GB

Argonne Leadership Computing Facility

Radja Boughezal, ANL

Scalable NNLO Phenomenology
They will be replaced by even more powerful supercomputers in the near future (Aurora at Argonne, 18 times more powerful than Mira; Cori at NERSC)!
NNLO QCD in the Era of Supercomputers

• An impressive amount of computing resources is available to the users. But there is a price for that: your code must be structured to run on the supercomputers local architectures.

• Crucial for efficient run: your code must have a hybrid implementation of MPI+OpenMP protocols.
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• Crucial for efficient run: your code must have a hybrid implementation of MPI+OpenMP protocols.
Our NNLO code supports such a hybrid implementation of MPI+OpenMP. Strong scaling to the several-thousand nodes level!
NNLO QCD in the Era of Supercomputers

- Our NNLO code supports such a hybrid implementation of MPI+OpenMP nodes level!

\[ W+j, Z+j, H+j \] distributions obtained within hours!
Conclusions

• We have entered the era of percent-level jet phenomenology
• The N-jettiness subtraction scheme is a powerful method in predicting NNLO cross sections for jet production processes
• NNLO corrections to V+jet are at the percent level; ready for precision measurements at the LHC Run II
• NNLO results for Higgs+j makes us ready for continued exploration of the Higgs sector.
• We are at the point where standard computing with small clusters is not enough for precision physics. The use of supercomputers for NNLO calculations is a new paradigm!