PineAPPL interface to xFitter and MSR mass studies with MCFM

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NCBJ

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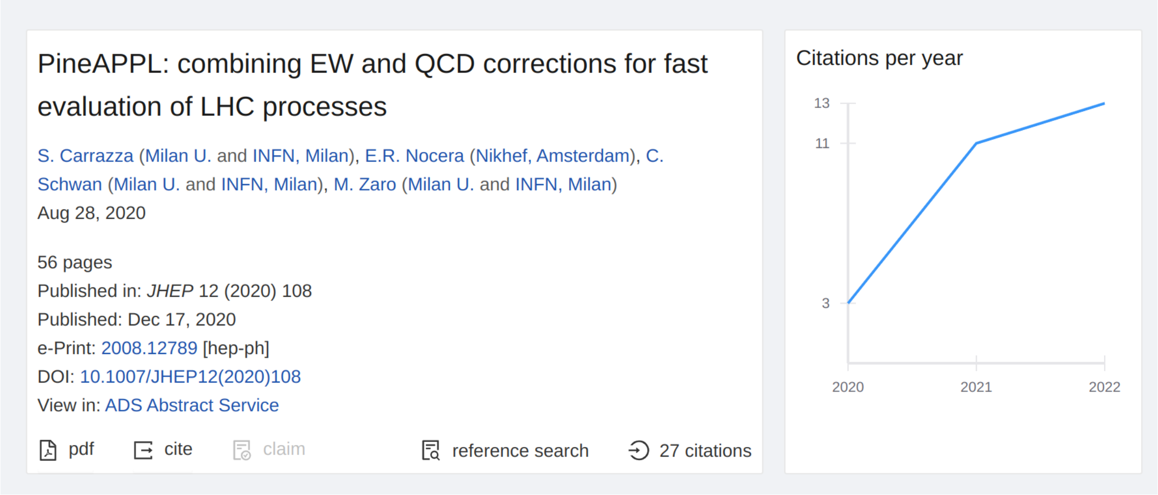
Introduction

- *Two-part talk*: **1st**, introducing **PineAPPL** to xFitter. **2nd**, observations of the behavior of the **top quark MSR mass**: *implications relevant to future experimental fits*
- **PineAPPL**: *a new type of interpolation grid*


PineAPPL: combining EW and QCD corrections for fast evaluation of LHC processes

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- Supports inclusion of QCD & EW corrections *in the grid*, to any fixed order
- Currently gaining popularity, linked to many codes
  - E.g. MadGraph5, SMEFT codes, YADISM, MATRIX...

See the talk by S. Kallweit!

Technical matters concerning PineAPPL

- PineAPPL code available at https://github.com/NNPDF/pineappl
- Written in Rust https://www.rust-lang.org
  - *Full* PineAPPL installation requires Rust compiler & package handlers cargo/cargo-c

See xFitter branch ready for merge, at
https://gitlab.cern.ch/fitters/xfitter/-/tree/pineappl

In the master **install script** after the merge:

- options for ***full installation*** or ***light installation*** with minimal deps: using precompiled pineappl files + a C interface

Installation

Pineappl branch merge currently waiting to be accepted. To install a backup *before* the merge, do:

```
wget https://gitlab.cern.ch/fitters/xfitter/-/raw/pineapplmaster/tools/install-xfitter
chmod +x install-xfitter
./install-xfitter pineapplmaster
~$
```

At the beginning of the script:

Relevant program version numbers

Include **full Rust installation** under deps? Quite heavy, and unnecessary if you have no use for a full standalone PineAPPL installation

Set to 0 to install PineAPPL! Flag included considering eventual merge with master, and PineAPPL considered “optional” for now

1: PineAPPL to be used only w/in xFitter. Set to **0** if you want to use also standalone PineAPPL features

```
## Programs versions
lhapdfver=6.5.1
hathorver=2.0
hoppetver=1.2.0
applgridver=1.6.32
qcdnumver=18-00-00
apfelver=3.0.6
apfelgridver=1.0.5
apfelxxver=4.0.0
dyturbover=1.2
pineapplver=0.5.8
rustver=1.66.0
cargocver=0.9.14

# skip some packages depending on xfitter version
skip_apfelgrid=0
skip_dyturbo=1
skip_rust=1
skip_pineappl=1
# fetch precompiled files for pineappl if possible
pineappl_lite=1
```

Usage

- In .dat file

```
TheoryType = 'expression'
TermType   = 'reaction'
TermName   = 'P'
TermSource = 'PineAPPL'
TermInfo   = 'GridName=path/to/grid.pineappl.lz4'
TheorExpr  = 'P'
```

- In parameters.yaml

```
byReaction:
  PineAPPL:
    muF: 1.0
    muR: 1.0
    PDG: 2212
    Norm: 0
    #OrderMask : "1,0,0"
    #LumiMask : "1,0,0"
```

E.g. convolute with proton PDFs

Normalize by bin widths? Default: no

Comment out to use all orders/contributions available in grid

Order mask – in case not all orders are to be used

- The grids can contain various orders in EW and QCD couplings, as well as logs of factorization and renormalization scales
- If standalone PineAPPL installed, check grid contents by

```
pineappl obl --orders [gridfile]
```

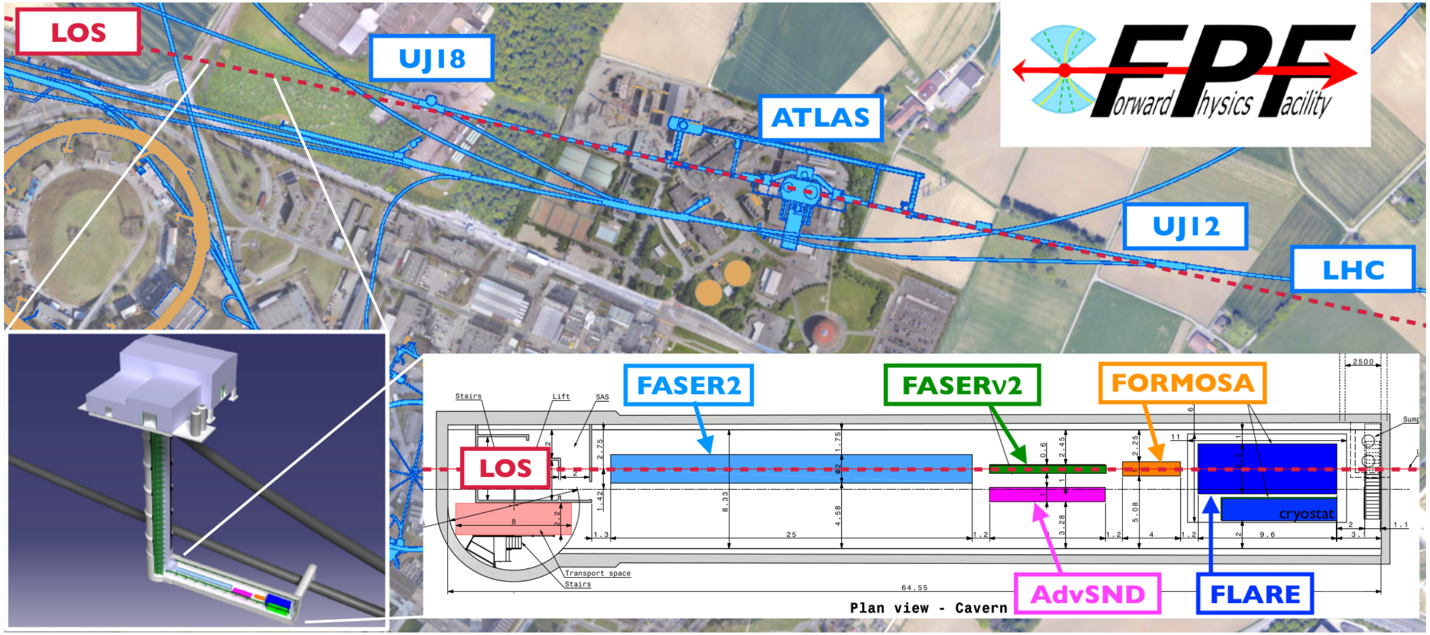
- Example: suppose the grid contents are

```
Orders={0,2,0,0,    //       alpha^2
        1,2,0,0,    //alphaS alpha^2
        1,2,0,1,};  //alphaS alpha^2 log xif^2
```

- ➔ E.g. to include LO only, the order mask parameter would be “1,0,0” (enable 1st line, disable the rest)
- ➔ N.B. order must be given via the mask, not read from constants.yaml!
- ➔ To ensure scale variations are performed properly, make sure to include also the relevant logs!

Application example
Neutrino DIS @ Forward Physics Facility FPF

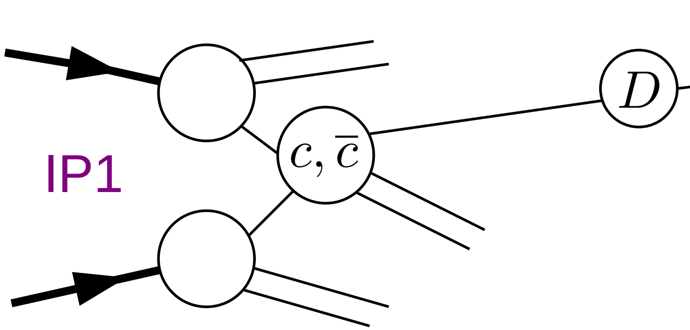
- A new facility proposed along the line-of-sight from IP1
  - Various experiments to detect e.g. forward neutrinos and BSM signals

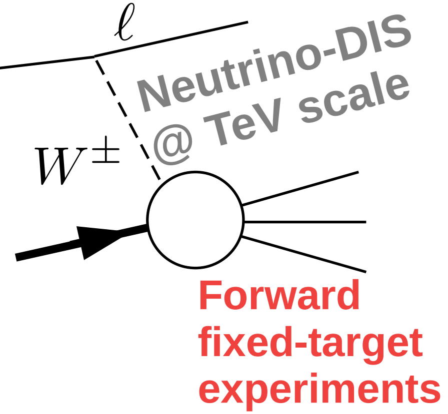


- Recall: the FASER collaboration recently reported 153^{+12}_{-13} observed neutrino events in 2303.14185 [hep-ex]
- With FPF, there is potential for e.g. constraining PDFs using neutrino-DIS
  - Also further physics questions can be investigated

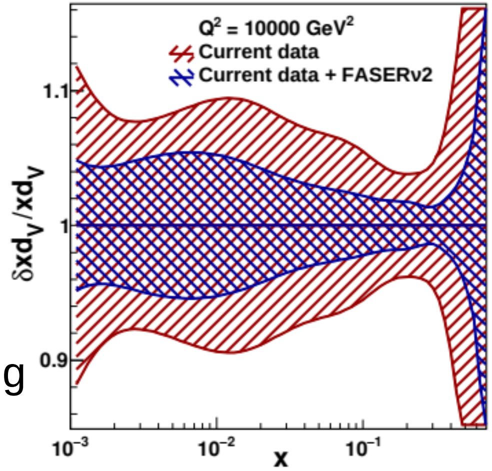
Application example
Neutrino DIS @ Forward Physics Facility FPF

- In principle could modify existing xFitter DIS codes. *However*, comparable studies performed by NNPDF collaborators, providing PineAPPL grids
  - PineAPPL abilities will be useful for xFitter users *in general* & increasingly beneficial in the near future





Preliminary profiling results assuming proton PDFs (PDF4LHC21) and accounting for statistical uncertainty estimates



Work-in-progress:
- More complete experimental uncertainty estimates
- Nuclear PDFs

Switching topics:

Behavior of the top quark MSR mass in $t\bar{t}$ pair invariant mass distribution at NLO

- Studies performed with MCFM v6.8 – independent of xFitter, but implications expected to be important for future fits of the top quark mass in running mass schemes
- See arXiv:2301.03546 [hep-ph], *submitted to Physics Letters B*

The running top quark mass

- The pole and $\overline{\text{MS}}$ masses are related by

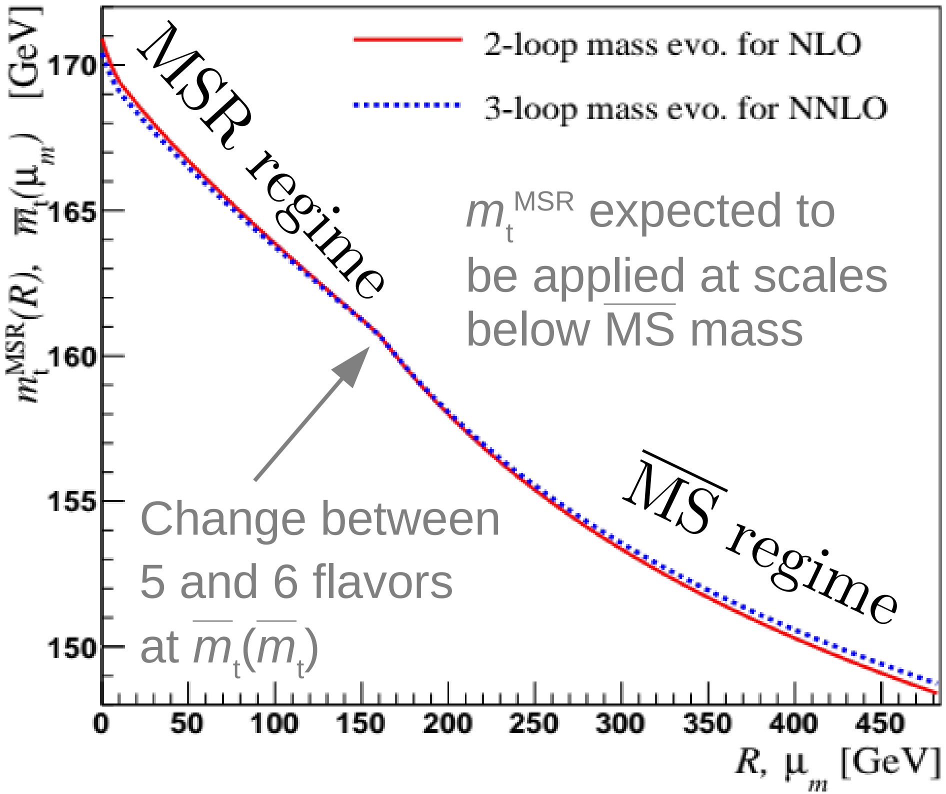
$$m_t^{\text{pole}} = \overline{m}_t(\mu_m) + \overline{m}_t(\mu_m) \sum_{n=1} \frac{\alpha_S(\mu_m)^n}{\pi^n} d_n(\mu_m)$$

- The $\overline{\text{MS}}$ mass has issues at the $t\bar{t}$ production threshold, unlike the pole mass

- **The MSR mass**: a mass renormalization scheme to bridge $\overline{\text{MS}}$ and pole masses

$$m_t^{\text{pole}} = m_t^{\text{MSR}} + R \sum_{n=1} \frac{\alpha_S(R)^n}{\pi^n} d_n^{\text{MSR}}(R)$$

- ***The behavior of the mass renormalization scale R is studied here for the first time***



The single-differential $t\bar{t}$ cross section at NLO

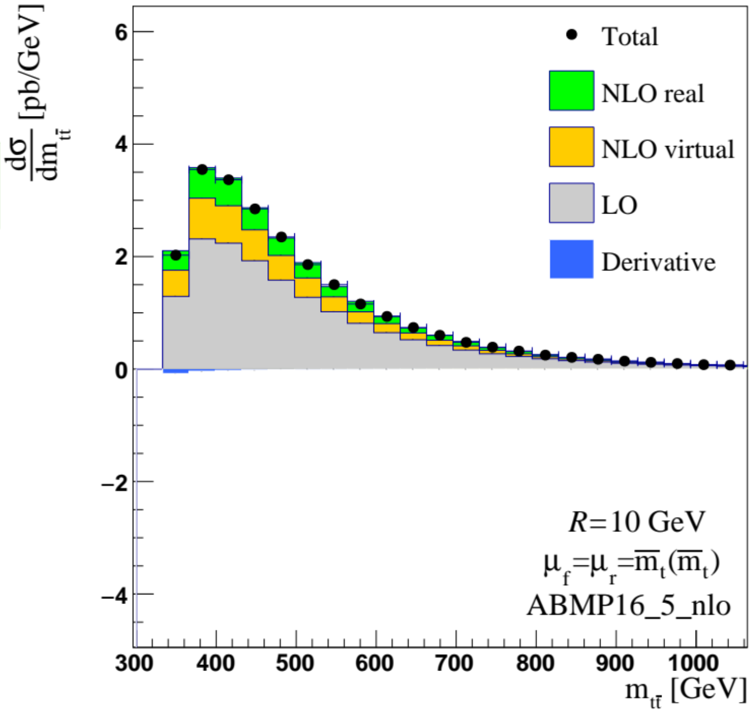
- In the MSR scheme, the cross section is divided into LO NLO and derivative terms

$$\frac{d\sigma}{dm_{t\bar{t}}} = a_S(\mu_r)^2 \frac{d\sigma^{(0)}}{dm_{t\bar{t}}}(m_t^{MSR}(R), \mu_r) + a_S(\mu_r)^3 \frac{d\sigma^{(1)}}{dm_{t\bar{t}}}(m_t^{MSR}(R), \mu_r) + a_S(\mu_r)^3 d_1 R \frac{d}{dm_t}\left(\frac{d\sigma^{(0)}(m_t, \mu_r)}{dm_{t\bar{t}}}\right)\Bigg|_{m_t = m_t^{MSR}(R)}$$

- Implemented into the MCFM v6.8 Monte Carlo
  - Also antiquark rapidity and p_T distributions available
  - Focus here on pair invariant mass distribution

Validated against:

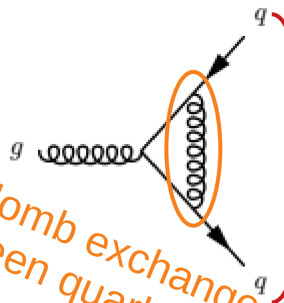
- Inclusive $t\bar{t}$ cross section implemented into HATHOR
- External differential computation translating pole scheme results to MSR



The single-differential $t\bar{t}$ cross section at NLO

Known issue

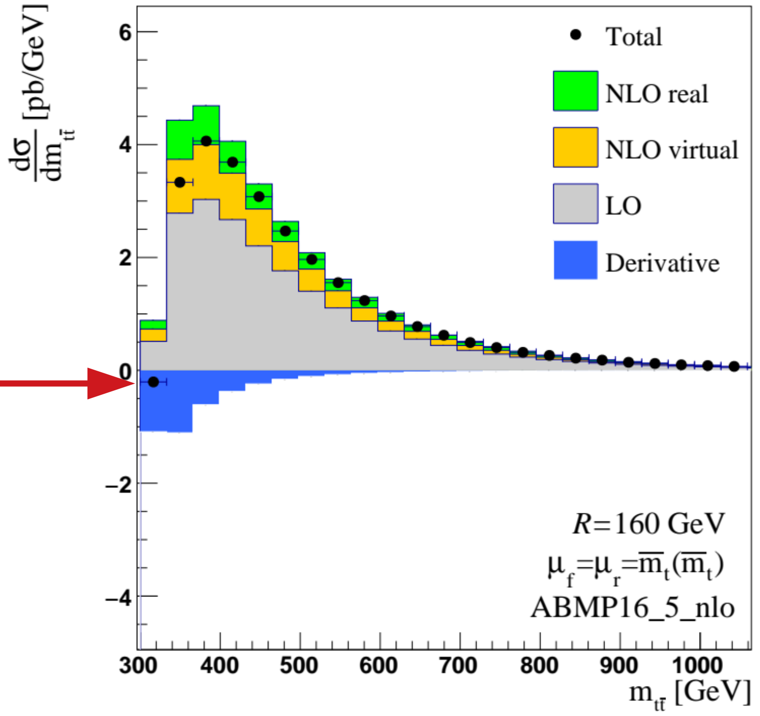
Fixed-order pQCD does not account for Coulomb effects at production threshold!



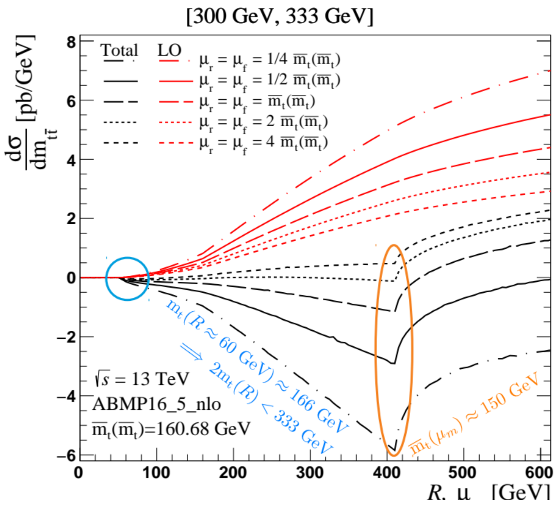
- **Multiscale problem**

  close to the pair production threshold, should be treated in non-relativistic QCD: $v << 1 \Rightarrow m_t >> p \sim m_t v >> E_K \sim ½ m_t v^2$

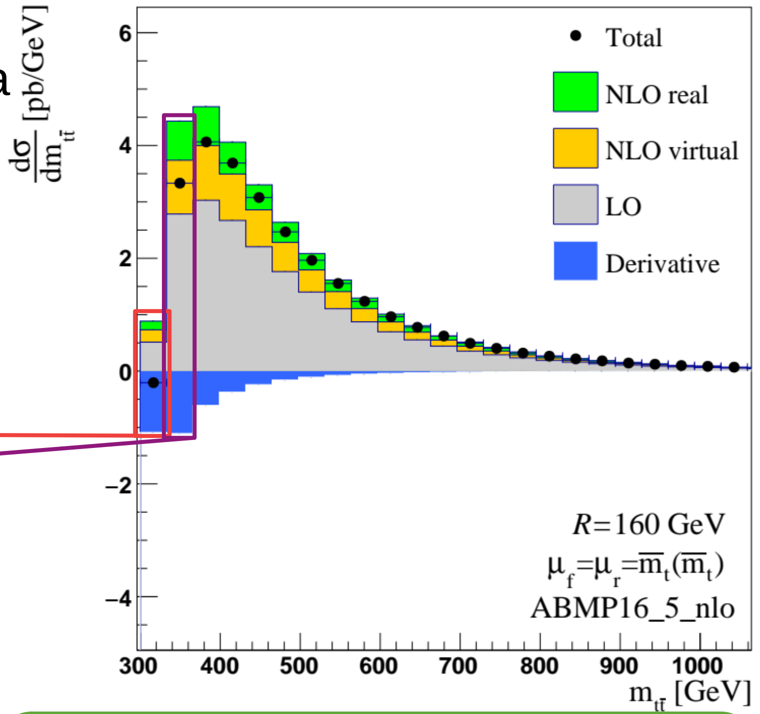
- Perturbative expansion in coupling breaks down
- Some theory work for corrections exists, but no computation is publicly available yet… so let's see what we can say about stability in fixed pQCD

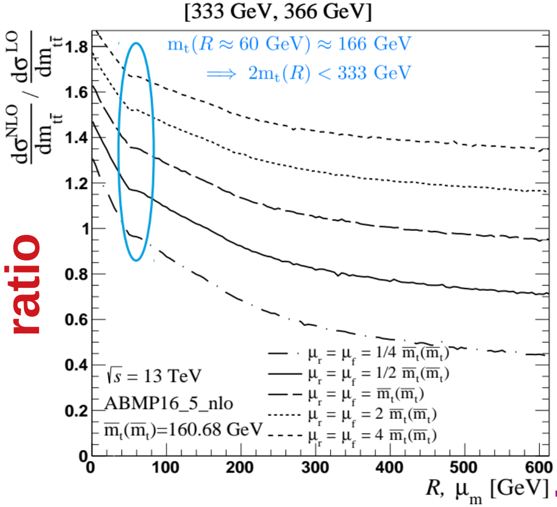


The single-differential $t\bar{t}$ cross section at NLO



- At the production threshold the derivative decreases faster as a function of R than other contributions increase
- At R > 410 GeV, m_t^{MSR} gets small, artificially pushing the threshold towards lower $m_{t\bar{t}}$





N.B. NLO/LO ratio

- Near the distribution peak, threshold effects also visible in the *ratio* of the full NLO cross section* to LO
  - Most sensitivity to m_t
- Stabilization at R > 60 GeV

Recommend to set $\mu_r = \mu_r = R$ = 80 GeV to increase robustness against scale variations

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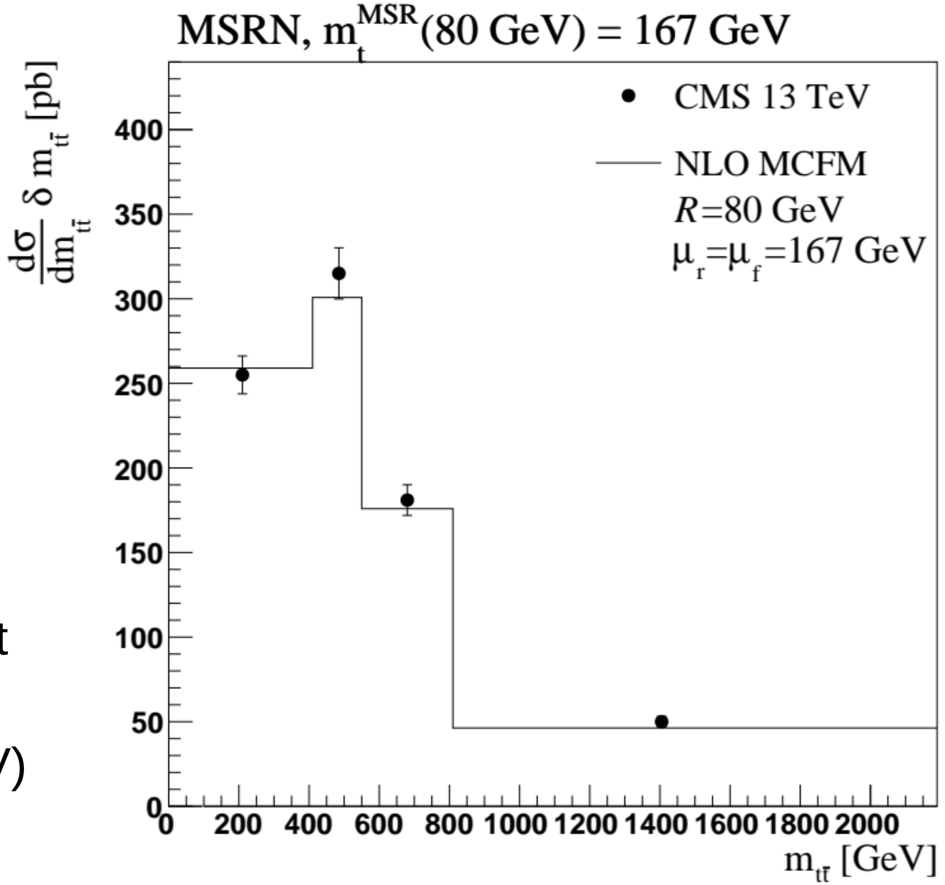
Extraction of the top quark MSR mass

- Using CMS $t\bar{t}$ cross section data measured as a function of $m_{t\bar{t}}$ at $\sqrt{s} = 13\ \mathrm{TeV}$ [doi:10.1016/j.physletb.2020.135263]

- Set R=80 GeV, scan for m_t^{MSR}(80 GeV)
  - For each mass, compute

$$\chi^2 = \sum_{i,j} (\sigma_i^{\mathrm{exp}} - \sigma_i^{\mathrm{th}}) C_{ij}^{-1} (\sigma_j^{\mathrm{exp}} - \sigma_j^{\mathrm{th}})$$

- Examine different scale choice options in different bins, also dynamical scales:
  - For $m_{t\bar{t}}$ < 420 GeV, set $\mu_r = \mu_r$ = ½ m_t^{MSR}(80 GeV)
  - For $m_{t\bar{t}}$ > 420 GeV, set $\mu_r = \mu_r = m_t^{MSR}$(80 GeV)

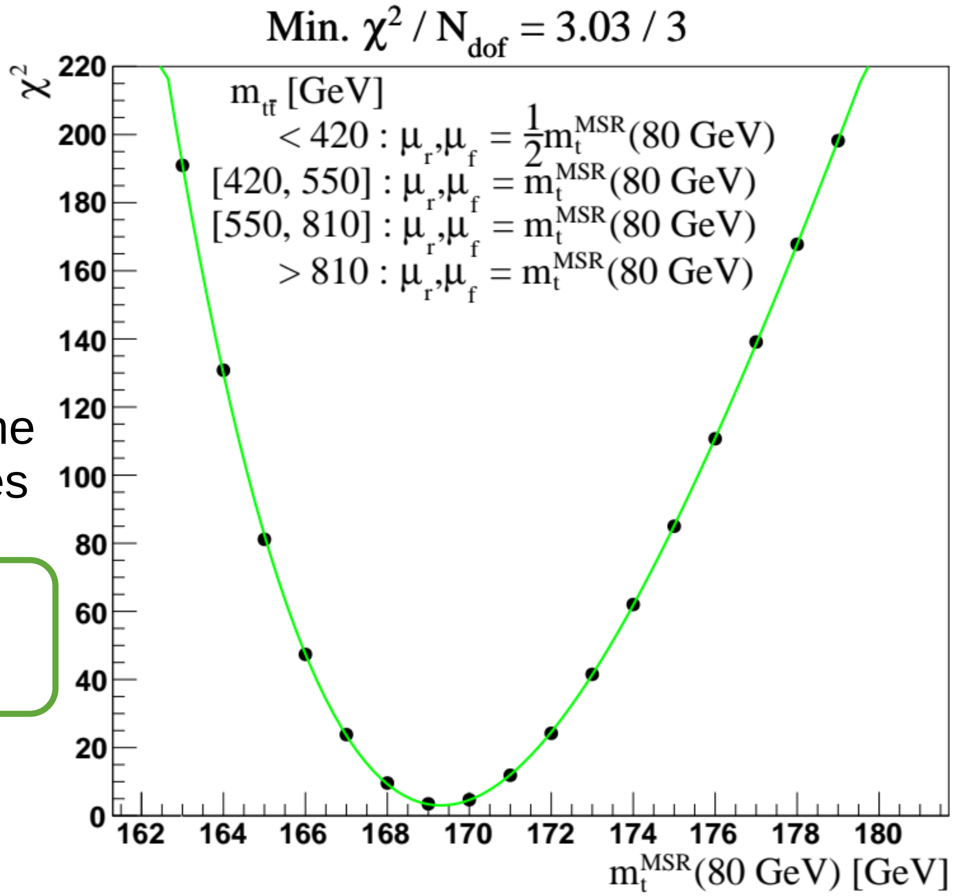


Extraction of the top quark MSR mass

- **Scale uncertainty**: variations of $\mu_r^{(i)}$, $\mu_f^{(i)}$,

- ***R*-uncertainty**: extracted $m_t^{\mathrm{MSR}}(80\ \mathrm{GeV})$ evolved to reference scales (e.g. R = 1 GeV) for comparison with other results

  Redo fits with R = 60 GeV and 100 GeV, take the difference in masses evolved to reference scales



With dynamical scale

$$m_t^{\mathrm{MSR}}(80\ \mathrm{GeV}) = 169.3 \pm 0.5\,(\mathrm{fit})^{+0.2}_{-0.4}\,(\mu_r,\mu_f)^{+0.2}_{-0.3}\,(R)\ \mathrm{GeV}$$

Without dyn. scale

$$m_t^{\mathrm{MSR}}(80\ \mathrm{GeV}) = 167.7 \pm 0.6\,(\mathrm{fit})^{+0.4}_{-0.6}\,(\mu_r,\mu_f)^{+0.4}_{-0.5}\,(R)\ \mathrm{GeV}$$

Dynamical scales increase precision

Extraction of the top quark MSR mass

- The extracted mass can be evolved to any reference scale:

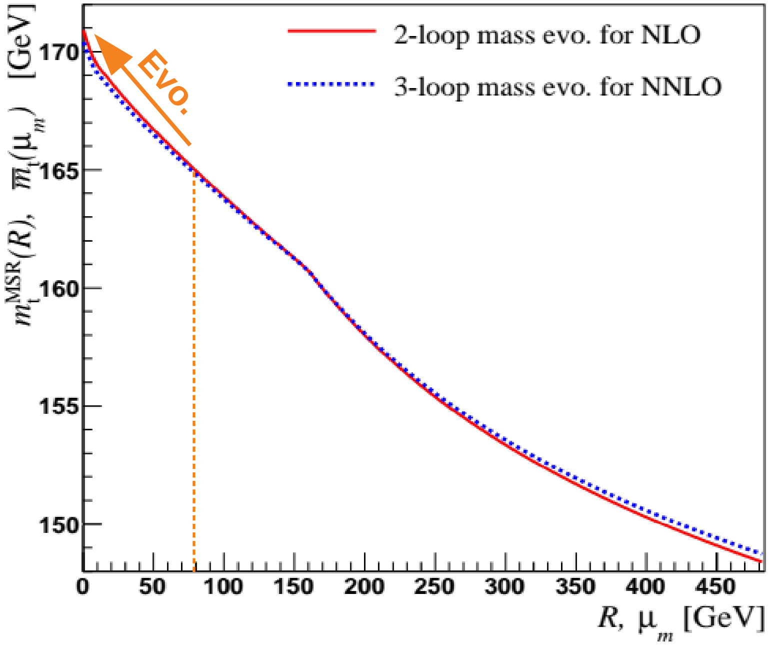
$$m_t^{\mathrm{MSR}}(80\ \mathrm{GeV}) = 169.3 \pm 0.5\,(\mathrm{fit})^{+0.2}_{-0.4}\,(\mu_r,\mu_f)^{+0.2}_{-0.3}\,(R)\ \mathrm{GeV}$$

R slightly above 1 GeV expected to become important checks for future analyses due to stability of $\alpha_s(\mu)$ at higher loop orders

$$m_t^{\mathrm{MSR}}(3\ \mathrm{GeV}) = 174.5 \pm 0.5\,(\mathrm{fit})^{+0.2}_{-0.4}\,(\mu_r,\mu_f)^{+0.2}_{-0.3}\,(R)\ \mathrm{GeV}$$

$$m_t^{\mathrm{MSR}}(1\ \mathrm{GeV}) = 174.8 \pm 0.5\,(\mathrm{fit})^{+0.2}_{-0.4}\,(\mu_r,\mu_f)^{+0.2}_{-0.3}\,(R)\ \mathrm{GeV}$$

At low *R*, the MSR scheme approximates the pole mass



Extraction of the top quark MSR mass

- **Alternatively** compute cross section predictions with R=1 GeV, to extract m_t^{MSR}(1 GeV) instead of evolving m_t^{MSR}(80 GeV) to R=1 GeV afterwards
- **Result** $m_{\mathrm{t}}^{\mathrm{MSR}}(1\ \mathrm{GeV}) = 170.1 \pm 0.6\,(\mathrm{fit})^{+1.1}_{-0.9}\,(\mu_r, \mu_f)\ \mathrm{GeV}$
- This approach has been used in previous extractions of the top quark MSR mass
- The result is significantly lower than the suggested procedure, but agrees with previous results and pole mass results (after translation), e.g. [arXiv:1904.05237]:

$$m_{\mathrm{t}}^{\mathrm{pole}} = 170.5 \pm 0.8\ \ \mathrm{GeV}$$

- ***Underpins the importance of proper scale setting and procedures in future analyses!***

Take-home-message:

$m_{\mathrm{t,th}}^{\mathrm{MSR}}(80\ \mathrm{GeV})$ ↔ $\sigma(m_{\mathrm{t,th}}^{\mathrm{MSR}}(80\ \mathrm{GeV}))$ — ***Stability*** *w.r.t. scales*

$m_{\mathrm{t,th}}^{\mathrm{MSR}}(1\ \mathrm{GeV})$

Conventionally start here

$\sigma(m_{\mathrm{t,th}}^{\mathrm{MSR}}(1\ \mathrm{GeV}))$

$m_{\mathrm{t,extr.}}^{\mathrm{MSR}}(80\ \mathrm{GeV})$

$m_{\mathrm{t,extr.}}^{\mathrm{MSR}}(1\ \mathrm{GeV}) \neq m_{\mathrm{t,extr.}}^{\mathrm{MSR}}(1\ \mathrm{GeV})$

Approaches do not "commute"!

However, stability arguments expected to hold with more complete predictions

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Summary and outlook

- **Implemented PineAPPL interface to xFitter**
  - Applications to LHC analyses already underway, stay tuned!
  - Thanks to *C. Schwan, S. Amoroso, X. Shen* for discussion & feedback!

- **First study of *R*-scale behavior + extracting the top quark MSR mass**
  - Low μ_r, μ_f values near the production threshold + dynamical scale settings reduce uncertainties in top quark MSR mass determination
  - The value extracted from CMS data at 13 TeV:

$$\mathrm{m_t^{MSR}}(80\ \mathrm{GeV}) = 169.3^{+0.6}_{-0.7}\ \mathrm{GeV} \quad \rightarrow \quad m_\mathrm{t}^{\mathrm{MSR}}(1\ \mathrm{GeV}) = 174.8^{+0.6}_{-0.7}\ \mathrm{GeV}$$

  - The final word will require treatment of Coulomb effects, but findings expected to remain valid

Thanks for your attention!

Comparison to previous MSR results

- ATLAS has derived a value for $m_t^{MSR}(R = 1\text{ GeV})$ [ATL-PHYS-PUB-2021-034]. Their results are however not comparable because:
  - Compares QCD predictions at next-to-leading log to parton shower MC simulations
  - Assuming $m_t^{MC} = 172.5$ GeV.
  - Not based on experimental data and hence not comparable
- Garzelli *et al.* [JHEP 04 (2021) 043] have extracted $m_{\rm t}^{\rm MSR}(3\ {\rm GeV}) = 169.6^{+0.8}_{-1.1}\,(\mu_r,\mu_f)\ {\rm GeV}$
  - Some tension to our $m_{\rm t}^{\rm MSR}(3\ {\rm GeV}) = 174.5 \pm 0.5\,({\rm fit})^{+0.2}_{-0.4}\,(\mu_r,\mu_f)^{+0.2}_{-0.3}\,(\mu_r,\mu_f)\ {\rm GeV}$
    - Their cross section predictions are computed using $m_t^{MSR}(3\text{ GeV})$ (not evolving the extracted mass)
    - They simultaneously fit PDFs and α_S, the latter resulting in $\alpha_S(m_Z) = 0.1132^{+0.0023}_{-0.0018}$
      - Two standard deviations away from the ABMP16 fit value at NLO, assumed by us