Precision QCD predictions with NNLO calculations

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Part I:

NNLO calculations: status and prospects

Indeed,

it is all about

Stress-testing the Standard Model at the LHC!

- Collider physics is complicated!
  - Many approaches are needed to probe it comprehensively
- I will focus on one aspect: NNLO QCD calculations.
- Is NNLO big deal?
  - Yes! But not as much as it was just few years ago!
- Reason:
  - Multitude of approaches and calculations made it possible to compute all 2-to-2 LHC processes very fast.
  - Only jets@NNLO is still outstanding but clearly it is only a matter of (short) time.

NNLO approaches (1)

- First were Smith, van Neerven and co.

  [Drell-Yan, e+e-] through mid-’90’s

- Early modern work was analytic (elegant but couldn’t cope with less-inclusive observables)

  [Higgs, Drell-Yan] Anastasiou, Dixon, Melnikov Petriello ’01-04

- Early numeric work based on sector decomposition (lead to tremendous progress; implementation is process dependent)

  Binoth and Heinrich ’04
  [Higgs, Drell-Yan] Anastasiou, Melnikov, Petriello ’03

- Antenna subtraction (ongoing progress)

  [e+e- → 3 jets] Weinzierl '08-09
  Gerhmann-De Ridder, Gehrmann, Glover, Heinrich ’07
  [dijets] Currie, Gehrmann-De Ridder, Gerhmann, Glover, Pires, Wells ’13-15
  [H+j] Chen, Gehrmann, Glover, Jacquier ’14
  [Z+j] Gehrmann-De Ridder, Gerhmann, Glover, Huss, Morgan ’15
  [tt (quarks)] Abelof, Gehrmann-De Ridder ’14

- Colorful subtraction (promising development)

  del Duca, Somogyi, Trocsanyi ’05
  [Higgs → bb] del Duca, Duhr, Somogyi, Tramontano, Trocsanyi ’15
  [e+e- → 3j] del Duca, Duhr, Kardos, Somogyi, Trocsanyi ‘16

NNLO approaches (2)

- q_T-subtraction
  - elegant and effortless for colorless final states:

Catani, Grazzini ‘07
[γγ] Catani, Cieri, de Florian, Ferrara, Grazzini ’11
[Wγ, Zγ] Grazzini, Kallweit, Rathlev,Torre ’13-15
[ZH] Ferrara, Grazzini, Tramontano ’14
[WH] Ferrara, Grazzini, Tramontano ’11-13
[WW] Gehrmann, Grazzini, Kallweit, Maierhoeffer,von Manteuffel,Pozzorini, Rathlev, Tancredi ’14
[ZZ] Cascioli, Gehrmann, Grazzini, Kallweit, Maierhoeffer, von Manteuffel,Pozzorini, Rathlev, Tancredi, Weihs ’14

  - being developed for general final states:

Zhu, Li, Li, Shao, Yang ‘12
Catani, Grazzini, Torre ’14
[tt-offdiagonal] Bonciani, Catani, Grazzini, Sargsyan, Torre ’15

- N-jettiness (new and very promising development) → See talks by R. Boughezal, F. Petriello

Gaunt, Stahlhofen, Tackmann, Walsh, '15
[Vj] Boughezal, Focke, Liu, Petriello ’15-16
[Zj] Boughezal, Focke, Giele, Liu, Petriello ’15
[Hj] Boughezal, Campbell, Ellis, Focke, Giele, Liu, Petriello ’15
[γγ] Campbell, Ellis, Li, Williams ‘16

NNLO approaches (3)

- Sector-improved residue subtraction

Czakon ‘10-11
Czakon, Heymes ‘14
Boughezal, Melnikov, Petriello, '11
[tt] Barnreuther, Czakon, Fiedler, Heymes, Mitov ’12-16
[Hj] Boughezal, Caola, Melnikov, Petriello, Schulze, '13-15
[B-decay] Caola, Czernecki, Liang, Melnikov, Szafron, '14
[t-decay] Brucherseifer, Caola, Melnikov, '13

- Future developments within this approach:
  - Independent implementation in a new code *STRIPPER*

    Czakon, Heymes, van Hameren

  - Process-independent (currently used for top production; adding top decay)
  - Important stability and numerics-related improvements being implemented
  - Linked to fastNLO: could output tables for any process
    - ✓ Very useful for pdf studies

      Britzger, Rabbertz, Sieber, Stober, Wobisch

NNLO with *STRIPPER*: the idea

- All integrations involving real radiation are done numerically
- All inputs are analytic. Only the minimal input is needed:
  - Tree-level amplitudes for RR
  - One-loop amplitudes for RV:
    - Finite parts
    - Singular limits (which are universal)
- Method is exact (basically this is the subtraction method at NNLO)
- Logic is simple:
  - IR singularities appear from soft/collinear radiation from external legs. They are universal.
  - Split the whole process into sum of terms, each having one particular singularity:
    - At NLO:
      - ($1\to2$) splitting
    - At NNLO:
      - ($1\to3$) splitting, or
      - two NLO-like splittings: ($1\to2$) & ($1\to2$)

NNLO with *STRIPPER*: the idea

- The splitting is controlled by selector functions (FKS idea)

Frixione, Kunszt, Signer '95

- Introduce a decomposition of unity:
  - An example at NLO:

$$\sum_{ik} \mathcal{S}_{i,k} = 1 \qquad \mathcal{S}_{i,k} = \frac{1}{D_1\, d_{i,k}}, \qquad D_1 = \sum_{ik} \frac{1}{d_{i,k}} \qquad d_{i,k} = \left(\frac{E_i}{\sqrt{\hat{s}}}\right)^{\alpha} (1-\cos\theta_{ik})^{\beta}$$

  - At NNLO:

$$\sum_{ij}\left[\sum_k \mathcal{S}_{ij,k} + \sum_{kl} \mathcal{S}_{i,k;j,l}\right] = 1 \qquad \mathcal{S}_{ij,k} = \frac{1}{D_2\, d_{ij,k}}, \qquad \mathcal{S}_{i,k;j,l} = \frac{1}{D_2\, d_{i,k} d_{j,l}}$$

$$D_2 = \sum_{ij}\left[\sum_k \frac{1}{d_{ij,k}} + \sum_{kl} \frac{1}{d_{i,k} d_{j,l}}\right].$$

$$d_{ij,k} = \left(\frac{E_i}{\sqrt{\hat{s}}}\right)^{\alpha_i} \left(\frac{E_j}{\sqrt{\hat{s}}}\right)^{\alpha_j} \left[(1-\cos\theta_{ij})(1-\cos\theta_{ik})(1-\cos\theta_{jk})\right]^{\beta}$$

- Selectors are such that they vanish in any singular limit different from the current one
- Introduce (same) parameterization but appropriate for each singular configurations

NNLO with *STRIPPER*: the idea

- At NLO, all that remains is to parameterize the energy and angle of the emitted parton and the singularirty is automatically factorized:

singular

$$\hat{\sigma}^{\mathrm{R}} = \sum_{ik} \iint_0^1 \frac{d\eta}{\eta^{1+\epsilon}} \frac{d\xi}{\xi^{1+2\epsilon}} f_{i,k}(\eta,\xi)$$

, where:

finite

$$f_{i,k}(\eta,\xi) = \frac{E_{\max}^2}{16\pi^3 \hat{s} N_{ab}} \left(\frac{\pi \mu_R^2 e^{\gamma_E}}{4E_{\max}^2(1-\eta)} \right)^{\epsilon} \int_{\mathcal{S}_1^{1-2\epsilon}} d\boldsymbol{\Omega}(\phi,\rho_1,\ldots) \int d\boldsymbol{\Phi}_n(p_1+p_2-u)\, \mathcal{S}_{i,k} \left[\eta\,\xi^2 \langle \mathcal{M}_{n+1}^{(0)} | \mathcal{M}_{n+1}^{(0)} \rangle \right] \mathrm{F}_{n+1}$$

Apply formula:

$$\frac{1}{x^{1+a\epsilon}} = -\frac{1}{a\epsilon}\delta(x) + \left[\frac{1}{x^{1+a\epsilon}}\right]_+ \qquad \int_0^1 dx \left[\frac{1}{x^{1+a\epsilon}}\right]_+ f(x) = \int_0^1 dx\, \frac{f(x)-f(0)}{x^{1+a\epsilon}}$$

Calculate limits:

$$\lim_{\eta\to 0}\left[\eta\,\xi^2 \langle \mathcal{M}_{n+1}^{(0)} | \mathcal{M}_{n+1}^{(0)} \rangle\right], \qquad \lim_{\xi\to 0}\left[\eta\,\xi^2 \langle \mathcal{M}_{n+1}^{(0)} | \mathcal{M}_{n+1}^{(0)} \rangle\right],$$

$$\lim_{\eta\to 0}\lim_{\xi\to 0}\left[\eta\,\xi^2 \langle \mathcal{M}_{n+1}^{(0)} | \mathcal{M}_{n+1}^{(0)} \rangle\right].$$

- At NNLO it is more complicated because we have overlapping singularities, i.e. no single parameterization will immediately work.

- Idea: use sector decomposition to disentangle the singularities   Czakon '10
  - Note: this is different from the original application of sector decomposition because here one parameterizes universal singularities (correspond to universal splittings)

NNLO with *STRIPPER*: the idea

- It turns out, it is sufficient to split the original integral in 5 terms, called sectors, that are dictated by the overlap of soft and collinear singularities in a 1→3 splitting.

- In each one of these 5 sectors one can now introduce a parameterization for the relevant 4 variables (2 energies and 2 angles) such that each sector has only factorized singularities!

- The relevant (singular) part of the PS integration reads:

$$\int \mathrm{d}\mathbf{\Phi}_{\text{unresolved}}\, \theta(u_1^0 - u_2^0) =$$

$$\left(\frac{\mu_R^2 e^{\gamma_E}}{4\pi}\right)^{2\epsilon} \int_{\mathcal{S}_1^{2-2\epsilon}} \mathrm{d}\mathbf{\Omega}(\theta_1,\phi_1,\rho_1,\ldots) \int_{\mathcal{S}_1^{2-2\epsilon}} \mathrm{d}\mathbf{\Omega}(\theta_2,\phi_2,\sigma_1,\sigma_2,\ldots) \int_0^{u^0_{\max}} \frac{\mathrm{d}u_1^0\,(u_1^0)^{1-2\epsilon}}{2(2\pi)^{3-2\epsilon}} \int_0^{u^0_{2\,\max}} \frac{\mathrm{d}u_2^0\,(u_2^0)^{1-2\epsilon}}{2(2\pi)^{3-2\epsilon}}\, \theta(u_1^0 - u_2^0) =$$

$$\frac{E^4_{\max}}{(2\pi)^6}\left(\frac{\pi\mu_R^2 e^{\gamma_E}}{8E^2_{\max}}\right)^{2\epsilon} \int_{\mathcal{S}_1^{1-2\epsilon}} \mathrm{d}\mathbf{\Omega}(\phi_1,\rho_1,\ldots) \int_{\mathcal{S}_1^{-2\epsilon}} \mathrm{d}\mathbf{\Omega}(\sigma_1,\sigma_2,\ldots) \int_0^1 \mathrm{d}\zeta\,\Big(\zeta(1-\zeta)\Big)^{-\frac{1}{2}-\epsilon} \iiiint_0^1 \mathrm{d}\eta_1 \mathrm{d}\eta_2 \mathrm{d}\xi_1 \mathrm{d}\xi_2 \sum_{i=1}^{5} \mu_{\mathcal{S}_i}\,,$$

- The relevant Jacobians for each of the 5 sectors:

	$\mu_{\mathcal{S}_i}$
$\mathcal{S}_1$	$\eta_1^{1-2\epsilon}\eta_2^{-\epsilon}\xi_1^{3-4\epsilon}\xi_2^{1-2\epsilon}\,((1-\eta_1)(2-\eta_1\eta_2))^{-\epsilon}\left(\frac{\eta_{31}(\eta_1,\eta_2)}{2-\eta_2}\right)^{1-2\epsilon}\xi_{2\,\max}^{2-2\epsilon}$
$\mathcal{S}_2$	$\eta_1^{2-3\epsilon}\eta_2^{1-2\epsilon}\xi_1^{3-4\epsilon}\xi_2^{1-2\epsilon}\,((1-\eta_2)(2-\eta_1\eta_2))^{-\epsilon}\left(\frac{\eta_{31}(\eta_2,\eta_1)}{2-\eta_1}\right)^{1-2\epsilon}\xi_{2\,\max}^{2-2\epsilon}$
$\mathcal{S}_3$	$\eta_1^{-\epsilon}\eta_2^{1-2\epsilon}\xi_1^{3-4\epsilon}\xi_2^{2-3\epsilon}\,((1-\eta_2)(2-\eta_1\eta_2\xi_2))^{-\epsilon}\left(\frac{\eta_{31}(\eta_2,\eta_1\xi_2)}{2-\eta_1\xi_2}\right)^{1-2\epsilon}\xi_{2\,\max}^{2-2\epsilon}$
$\mathcal{S}_4$	$\eta_1^{1-2\epsilon}\eta_2^{1-2\epsilon}\xi_1^{3-4\epsilon}\xi_2^{1-2\epsilon}\,((1-\eta_1)(2-\eta_2)(2-\eta_1(2-\eta_2)))^{-\epsilon}\,\eta_{32}^{1-2\epsilon}(\eta_1,\eta_2)\,\xi_{2\,\max}^{2-2\epsilon}$
$\mathcal{S}_5$	$\eta_1^{1-2\epsilon}\eta_2^{1-2\epsilon}\xi_1^{3-4\epsilon}\xi_2^{1-2\epsilon}\,((1-\eta_2)(2-\eta_1)(2-\eta_2(2-\eta_1)))^{-\epsilon}\,\eta_{32}^{1-2\epsilon}(\eta_2,\eta_1)\,\xi_{2\,\max}^{2-2\epsilon}$

- At this point proceed as we discussed at NLO

For full details see arxiv:1408.2500

The bottom line on NNLO calculations

- Good progress; makes us feel good
  - ✓ (Especially because another wish-list is completed ;)
- The questions we need to ask are:
  - What's the value of these result in terms of physics?
  - What's next on the to-do list?
- I'll address both in the following.

Out of the box NNLO's: how useful are they?

- Scales: important but importance perhaps underappreciated!

  (it was great that many of the discussion during the last few days involved scale choices!)

  - Fixing scales is just like developing new software:

    - Come up with an idea,
      - make it work,
        - make it optimized!

- How to store results and make them accessible and useable?

  - Plots in papers (not useful)

  - Electronic files (could be used, if nothing else available)

  - fastNLO, etc tables (convenient and fast; binning etc is rigid)

  - N-tuples - library of results (fully flexible but still non-existent)

NNLO: future needs and directions

- Establishing a connection between various processes:
  - Access all (many) processes under the same roof
- NLO is a good lead (although should not be followed verbatim due to computational cost at NNLO):
  - MCFM
  - MC@NLO
  - Powheg
  - Sherpa
  - …

Talk by: Walter Giele

- Matching NNLO to showers and description of realistic final states

Talks by: Stefan Hoeche
Christian Bauer

- Exploring new frontiers (beyond 2-to-2)
  - (Some of) the NNLO methods can in principle cope with any-multiplicity processes.
  - Numerics is however another issue…
  - However, no 2-loop amplitude is known beyond 2-to-2

Talks by: Gudrun Heinrich
Stefan Weinzierl

Part II:

NNLO precision applications

Choice of dynamic scales in top production

- Several tried and tested choices:

$$\mu_0 \sim m_t \ ,$$

$$\mu_0 \sim m_T = \sqrt{m_t^2 + p_T^2} \ ,$$

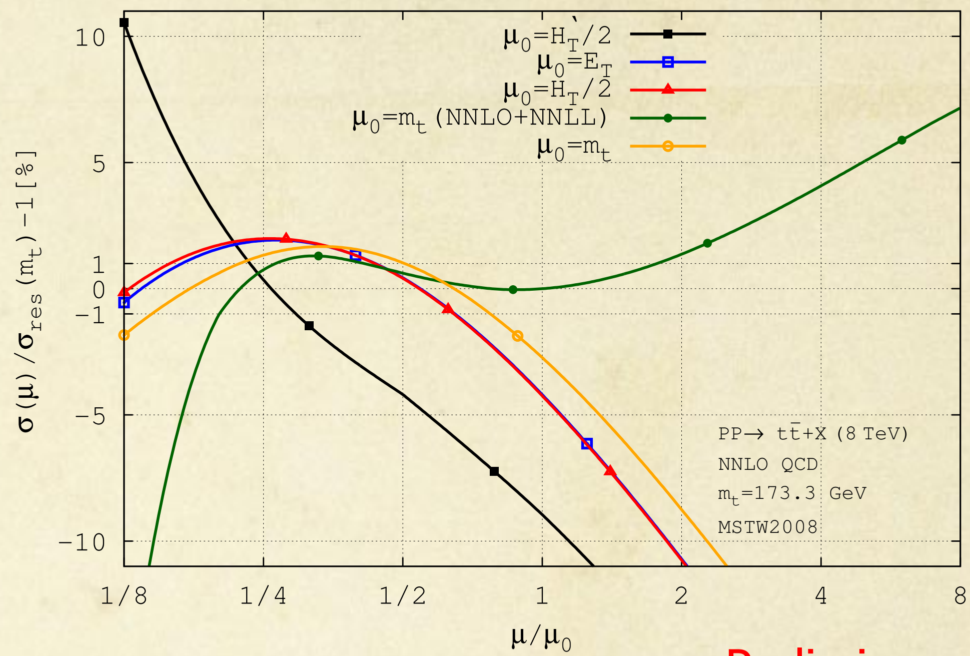
$$\mu_0 \sim H_T = \sqrt{m_t^2 + p_{T,t}^2} + \sqrt{m_t^2 + p_{T,\bar{t}}^2} \ ,$$

$$\mu_0 \sim H_T' = \sqrt{m_t^2 + p_{T,t}^2} + \sqrt{m_t^2 + p_{T,\bar{t}}^2} + \sum_i p_{T,i} \ ,$$

$$\mu_0 \sim E_T = \sqrt{\sqrt{m_t^2 + p_{T,t}^2}\sqrt{m_t^2 + p_{T,\bar{t}}^2}} \ ,$$

$$\mu_0 \sim H_{T,\text{int}} = \sqrt{(m_t/2)^2 + p_{T,t}^2} + \sqrt{(m_t/2)^2 + p_{T,\bar{t}}^2} \ ,$$

$$\mu_0 \sim m_{t\bar{t}} \ ,$$

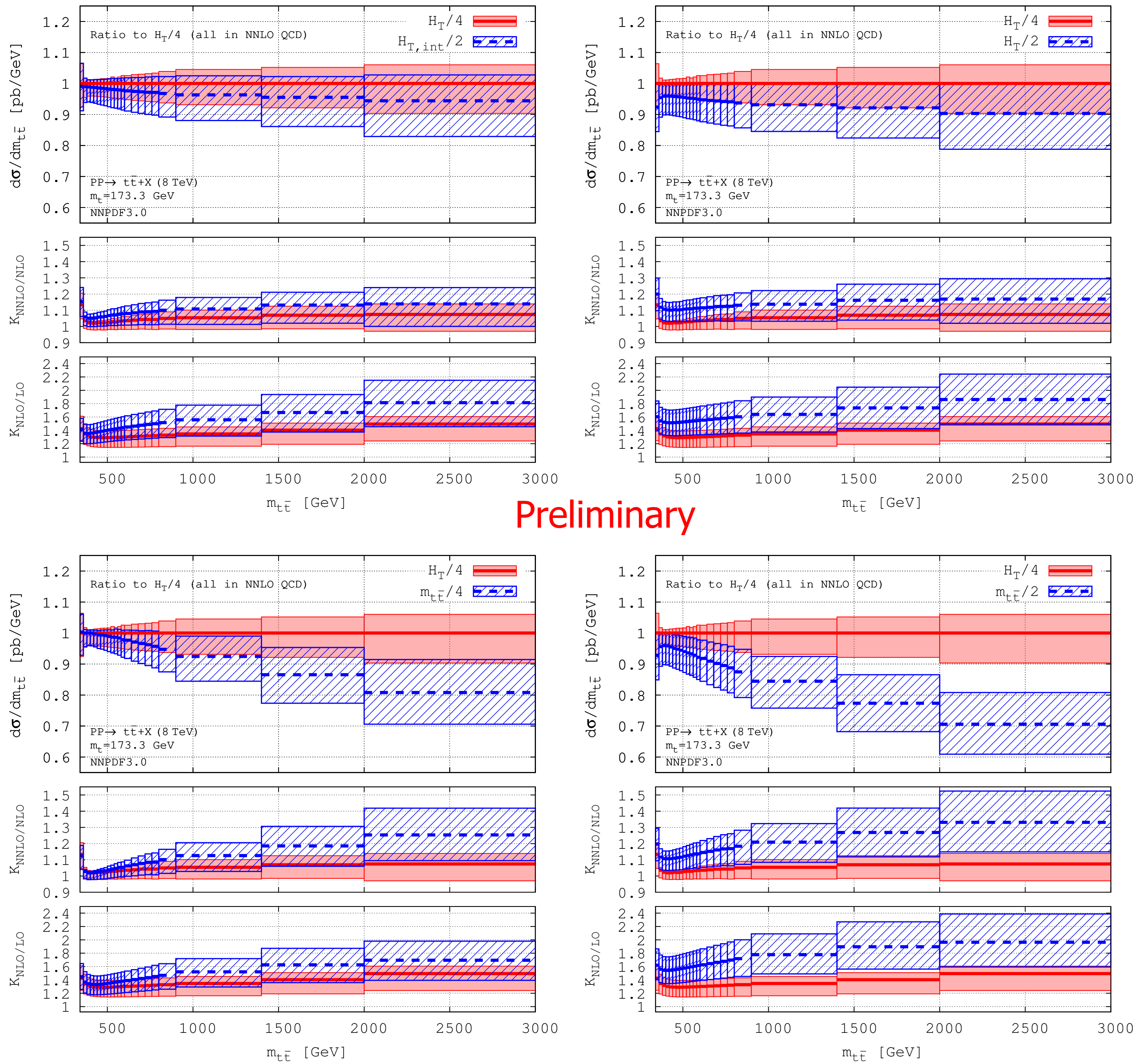


Preliminary

- What are we looking for here?
  - A scale that ensures fastest perturbative convergence (and agreement with data at low P_T, where lots of data is available and well understood)

$$\mu_0 = \begin{cases} \frac{m_T}{2} & \text{for :} \quad p_{T,t},\ p_{T,\bar{t}} \text{ and } p_{T,t/\bar{t}} \ , \\ \frac{H_T}{4} & \text{for :} \quad \text{all other distributions} \ . \end{cases}$$

NNLO differential with various dynamic scales (M_{tt} @ 8 TeV)



Preliminary

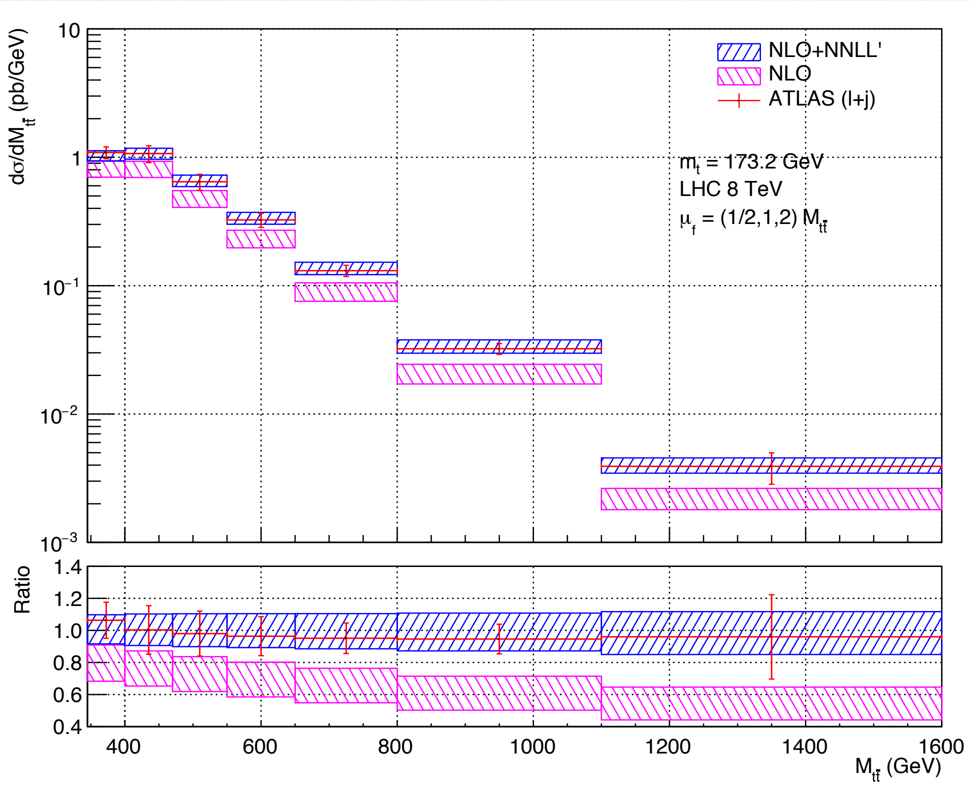
Czakon, Heymes, Mitov, to appear

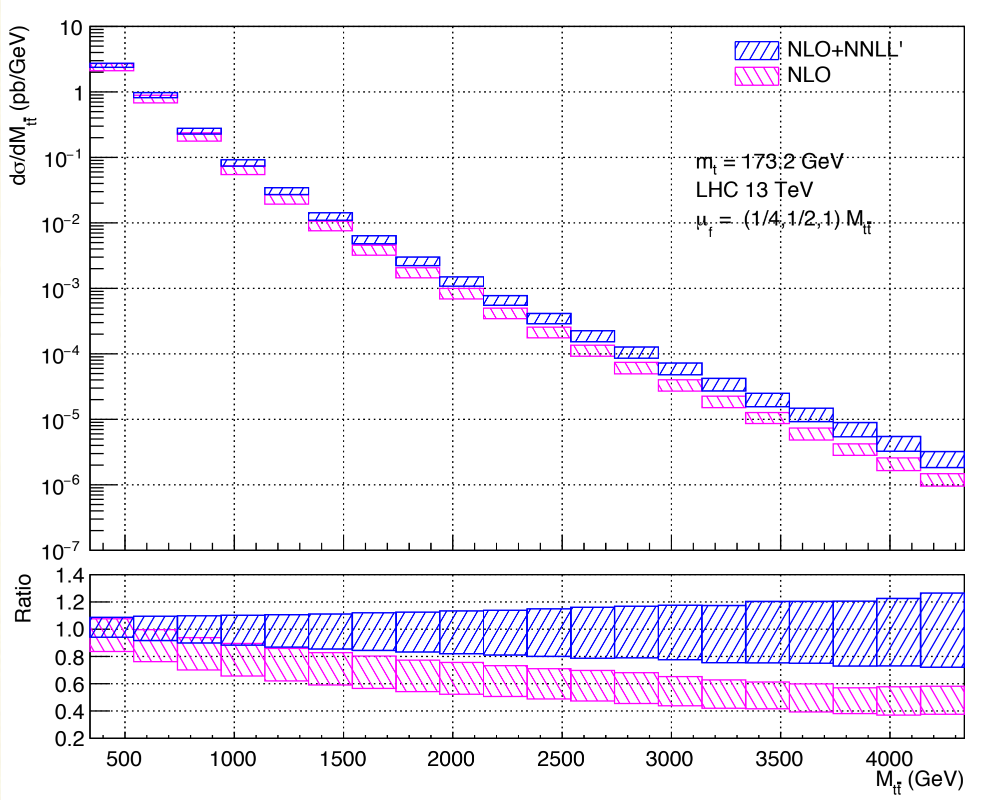
NNLO and scales: some lessons

- Lessons for the TEV range:

Recent result of NNLL resummation (soft and soft-collinear) of differential top production

Pecjak, Scottb, Wang, Yang arXiv:1601.07020v2





- Large difference between NLO and NLO + resummation may be an indication of suboptimal scale choice.

- Based on our study, perturbative convergence with M_{tt}-based scales is not optimal.

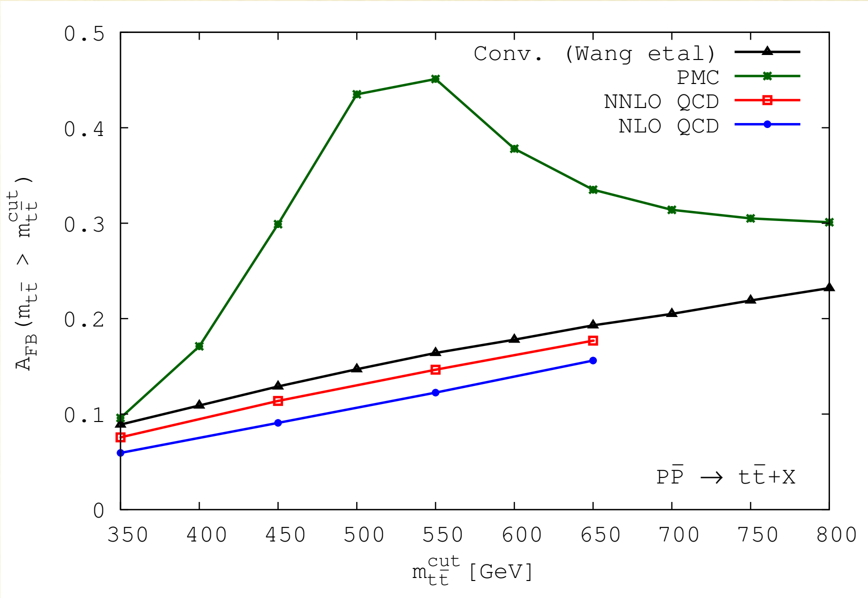
NNLO and scales: BLM/PMC

- At least one alternative to the usual scale setting exists
- Been applied to top production in a number of papers.

Wang, Wu, Si, Brodsky, Mojaza '12-15

- Example: top quark A_{FB} at the Tevatron

  - BLM/PMC versus usual scales (from arXiv:1601.05375v1)
  - Difference is simply huge!



- Recent application to Higgs physics

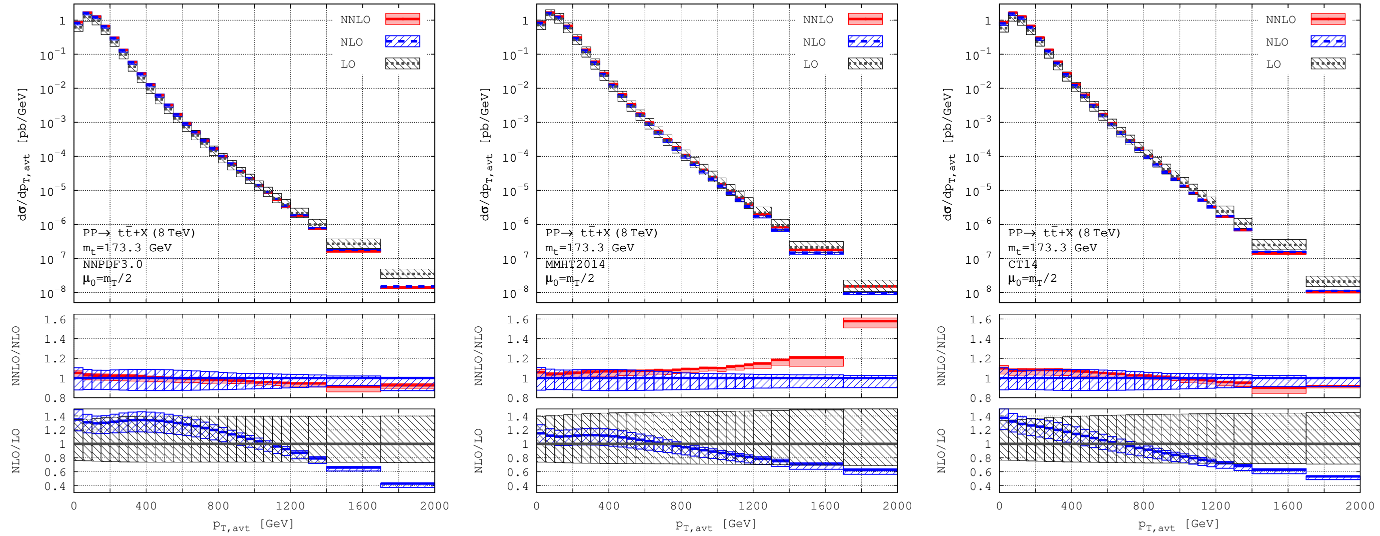
Wang, Wu, Brodsky, Mojaza '16

Precision NNLO applications: PDF's

- Precision predictions require pdf's.

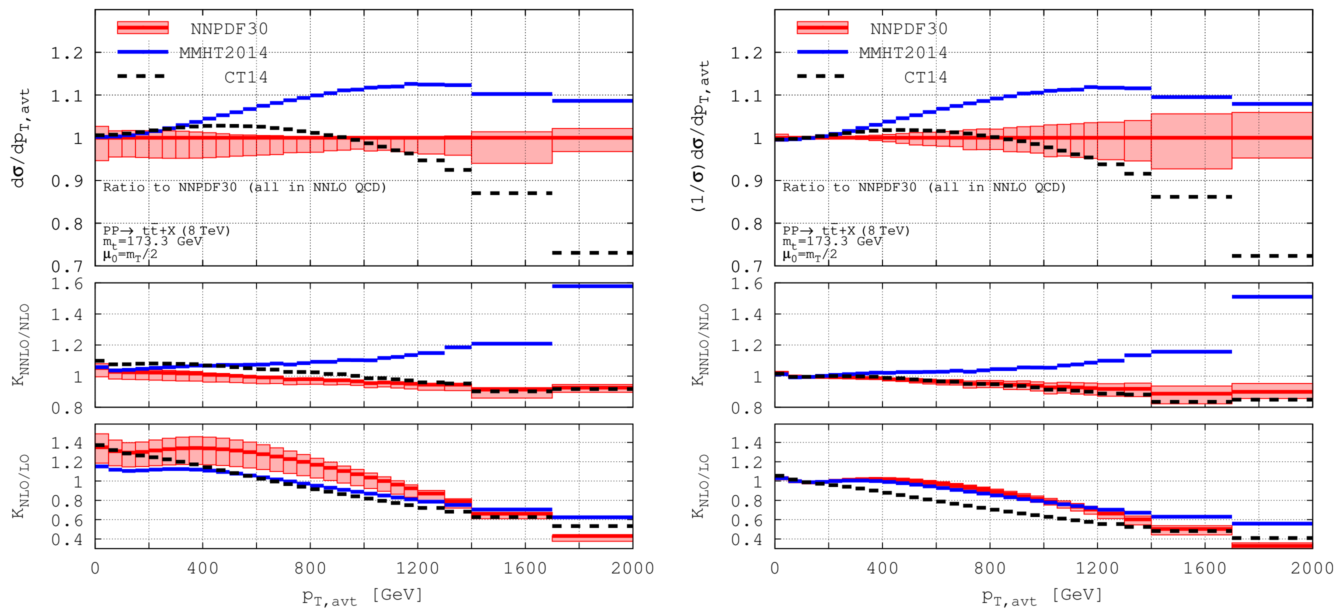
- Compare predictions based on different pdf sets (NNPDF3.0, CT14, MMHT2014):

- Absolute P_T distributions for each pdf set:



Preliminary

- Ratios of pdf sets (wrt NNPDF3.0):



Czakon, Heymes, Mitov, to appear

Precision NNLO applications: PDF's

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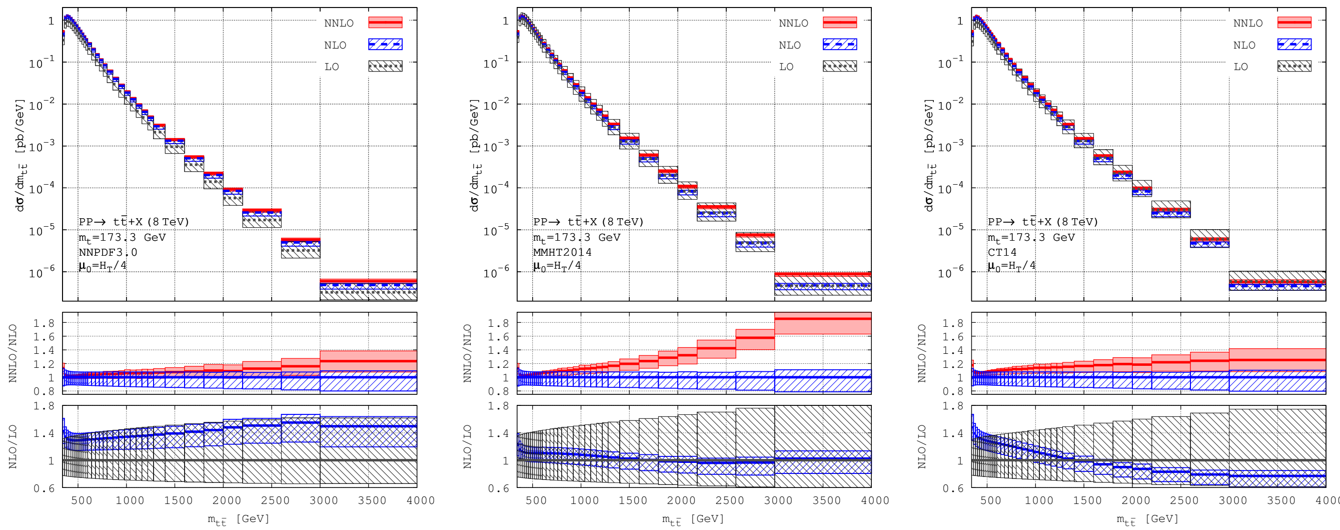

Preliminary

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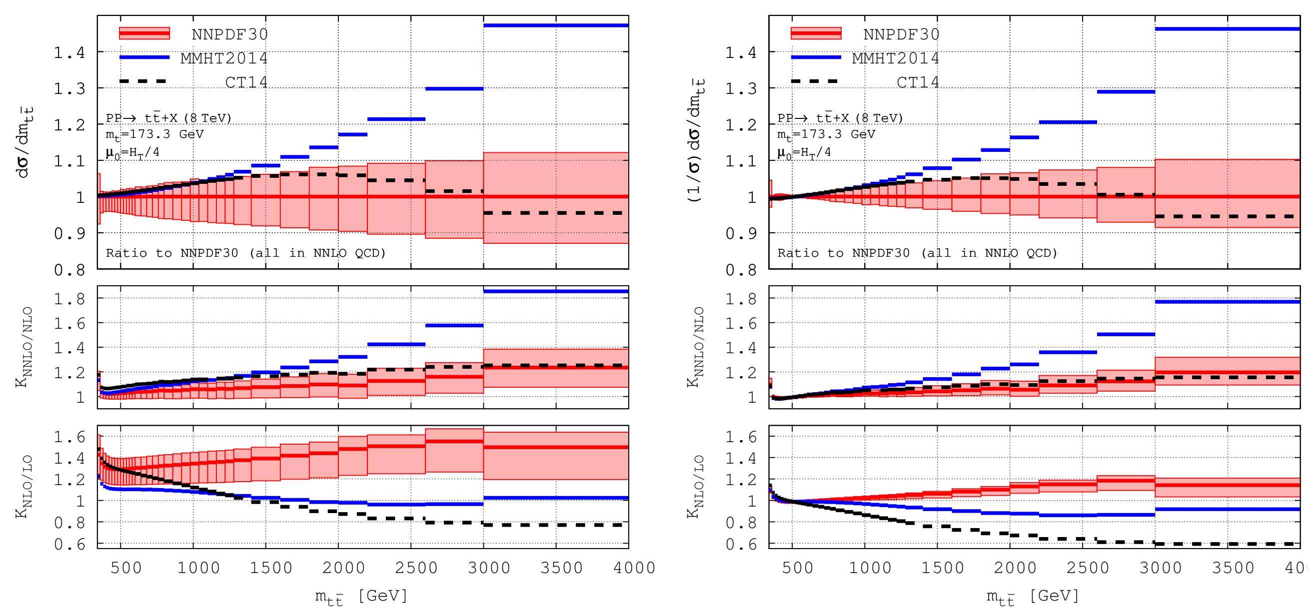
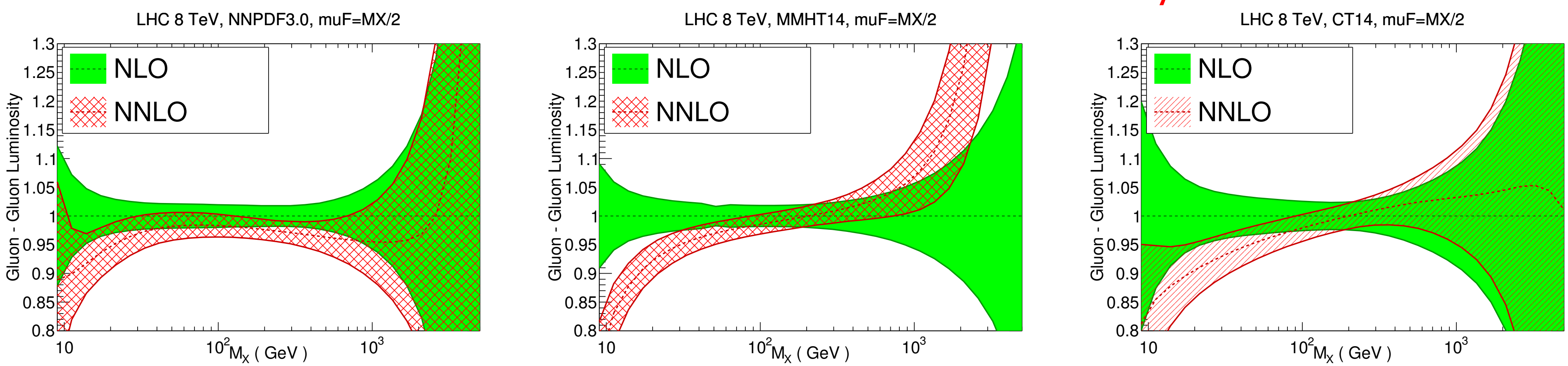


Czakon, Heymes, Mitov, to appear

Precision NNLO applications: PDF’s

- Understanding the large K-factors at NNLO:
  - a pdf effect – not scale related.

Preliminary



Czakon, Heymes, Mitov, to appear

Precision NNLO applications: PDF's

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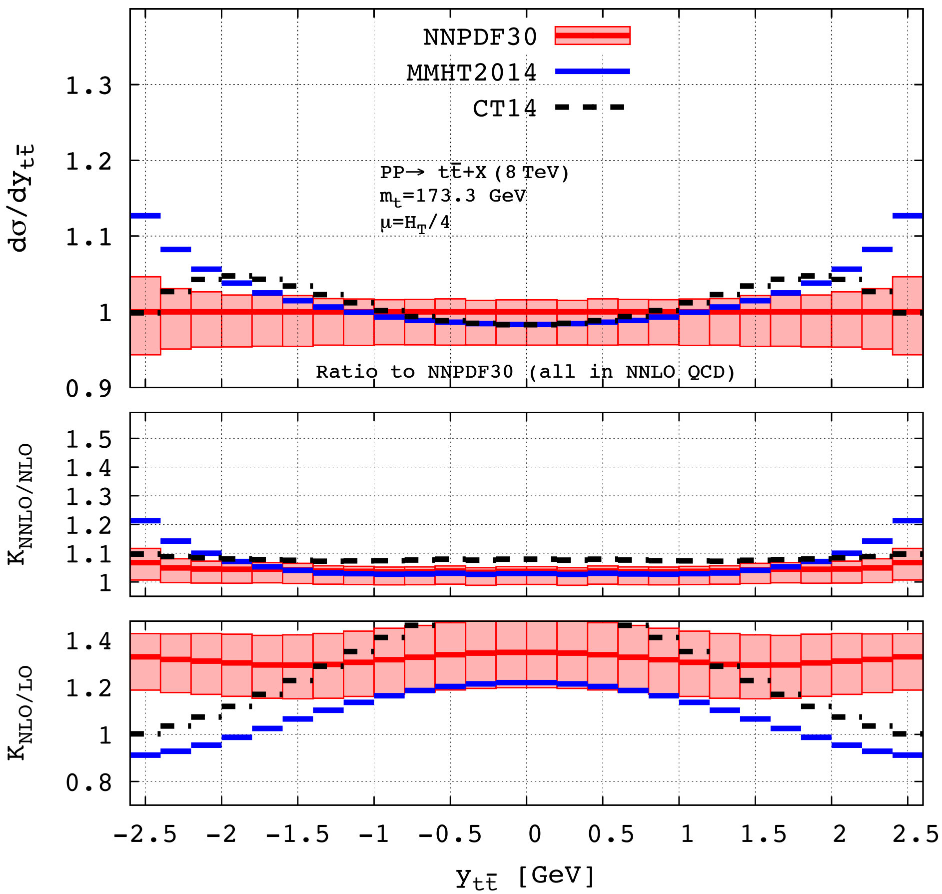
- And Y_{tt}:



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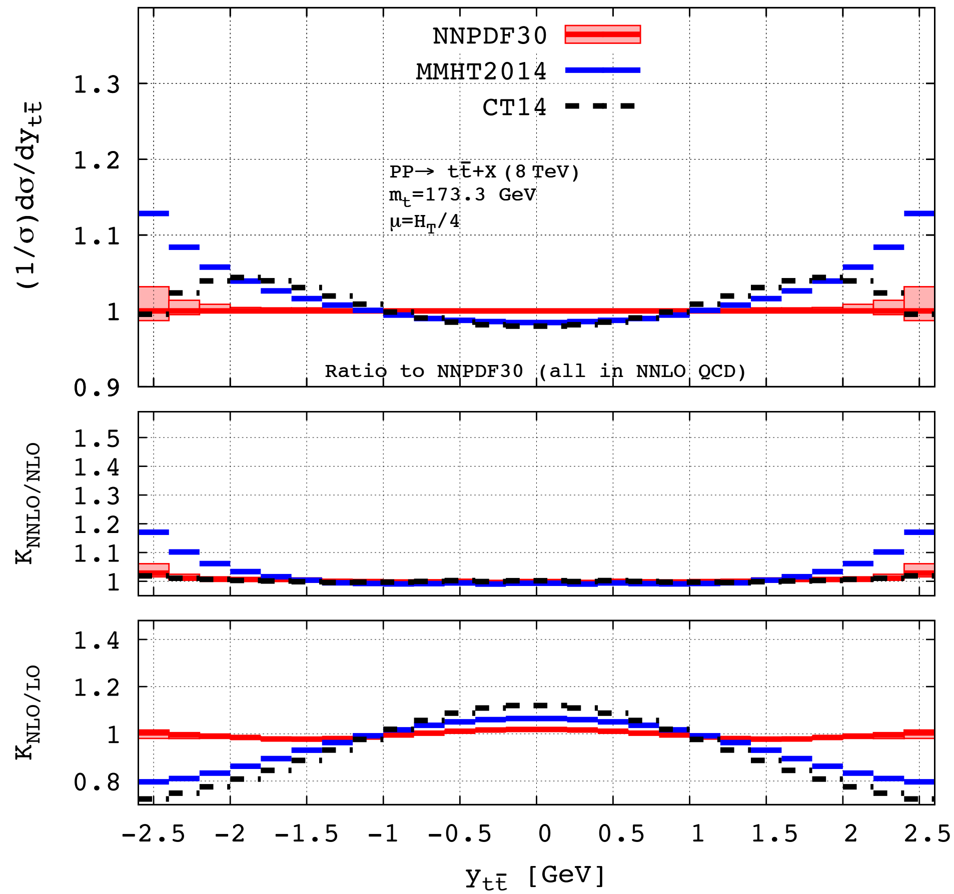


Czakon, Heymes, Mitov, to appear

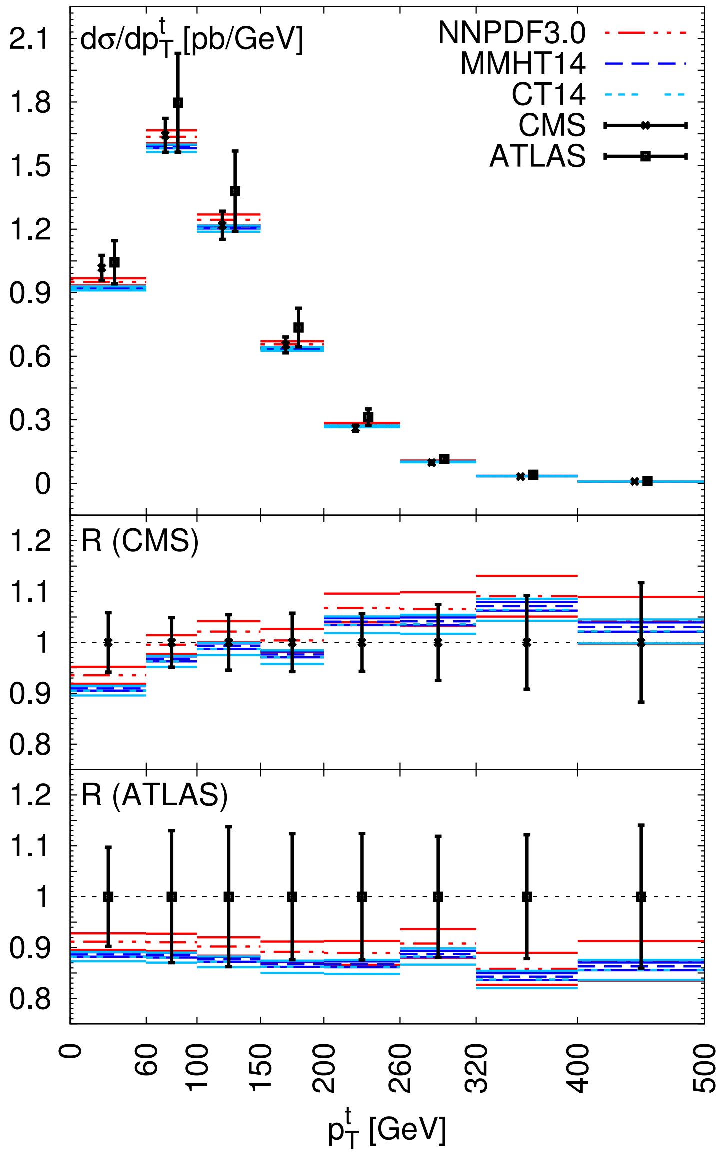
Precision NNLO applications: PDF's

- Clearly, we see strong dependence on the choice of pdf set
- This is very significant because it easily exceeds scale variation
- One way or another, top measurements offer the possibility to fix pdf's
  - In fact, it appears, precision progress in the TeV range will only be possible once improved pdf's appear.
- How much can we say about the pdf's from existing data (i.e. 8 TeV data)?

Fixing pdf's from existing top data

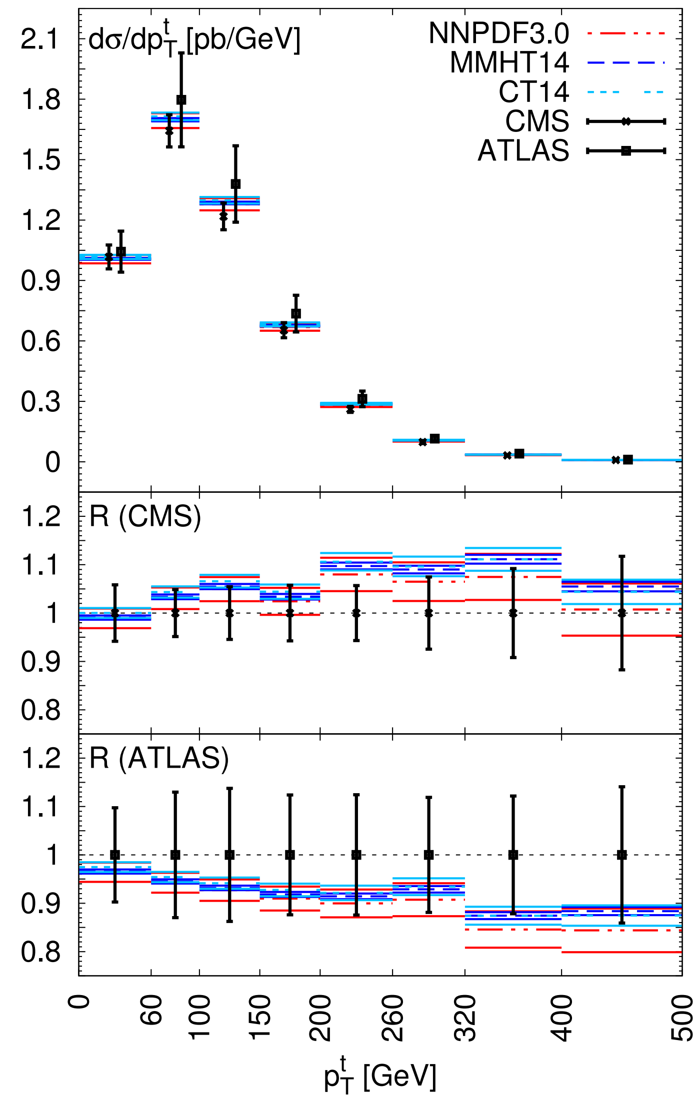
- Scale variation not included; only pdf error.

Absolute P_T: NLO



Preliminary

Absolute P_T: NNLO

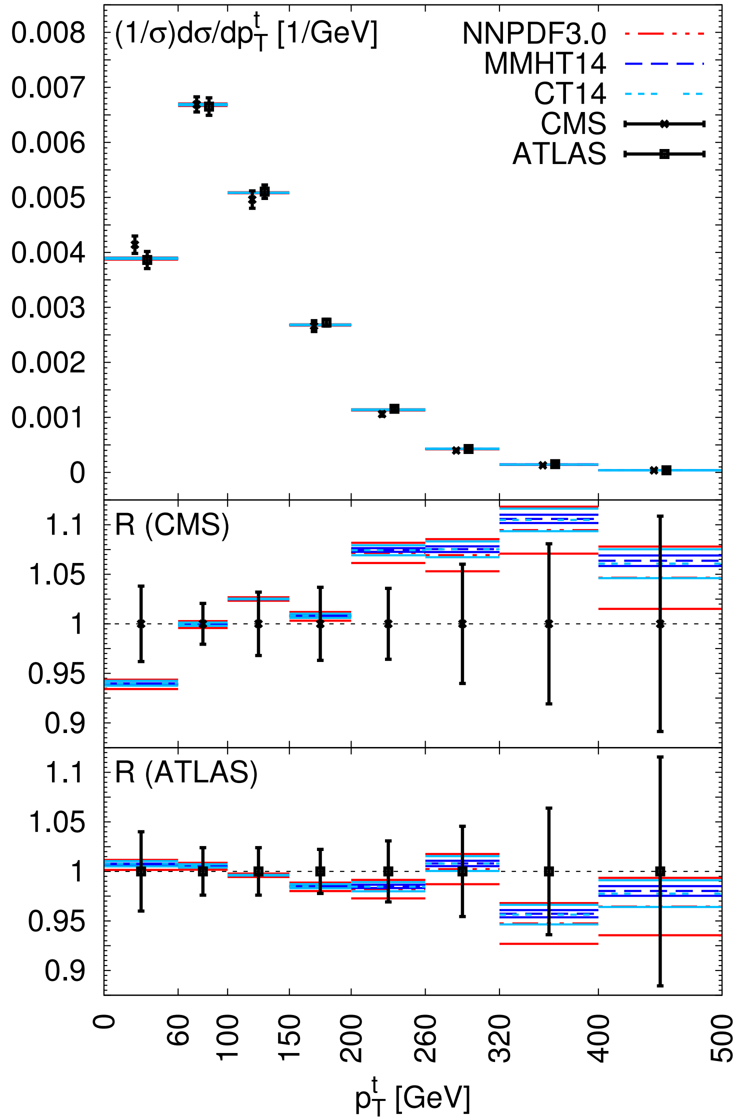


Hartland, Nocera, Rojo, Czakon, Mitov, to appear

Fixing pdf's from existing top data

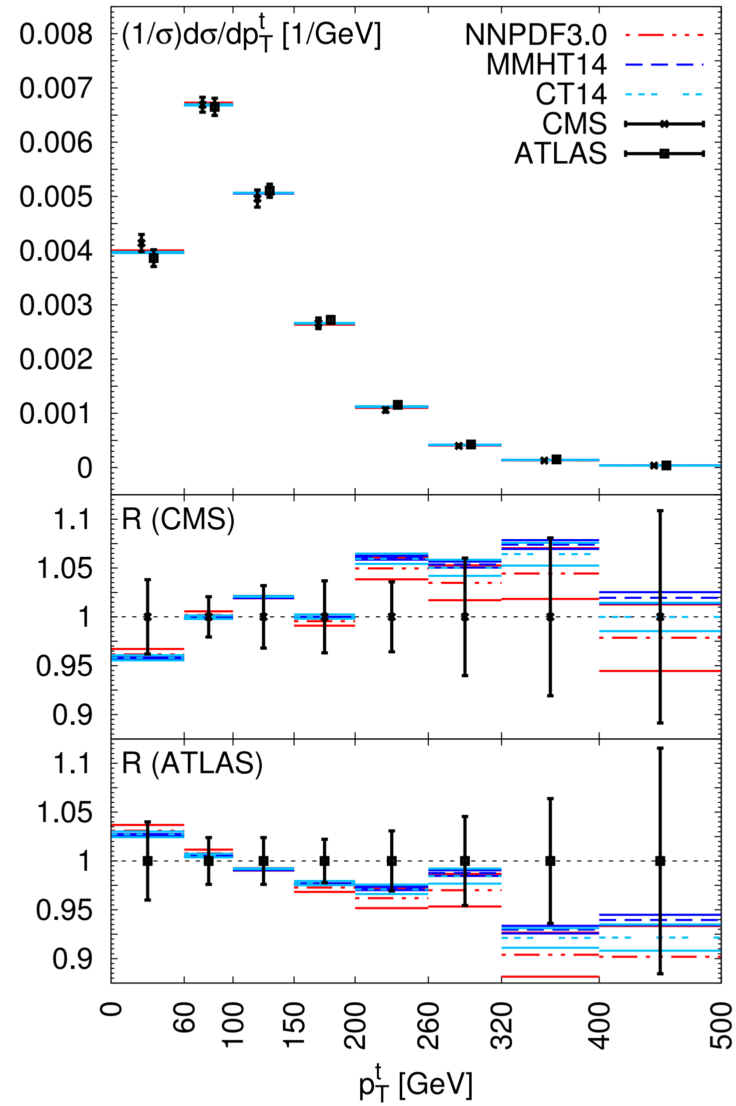
- Scale variation not included; only pdf error.

Normalized P_T: NLO



Preliminary

Normalized P_T: NNLO

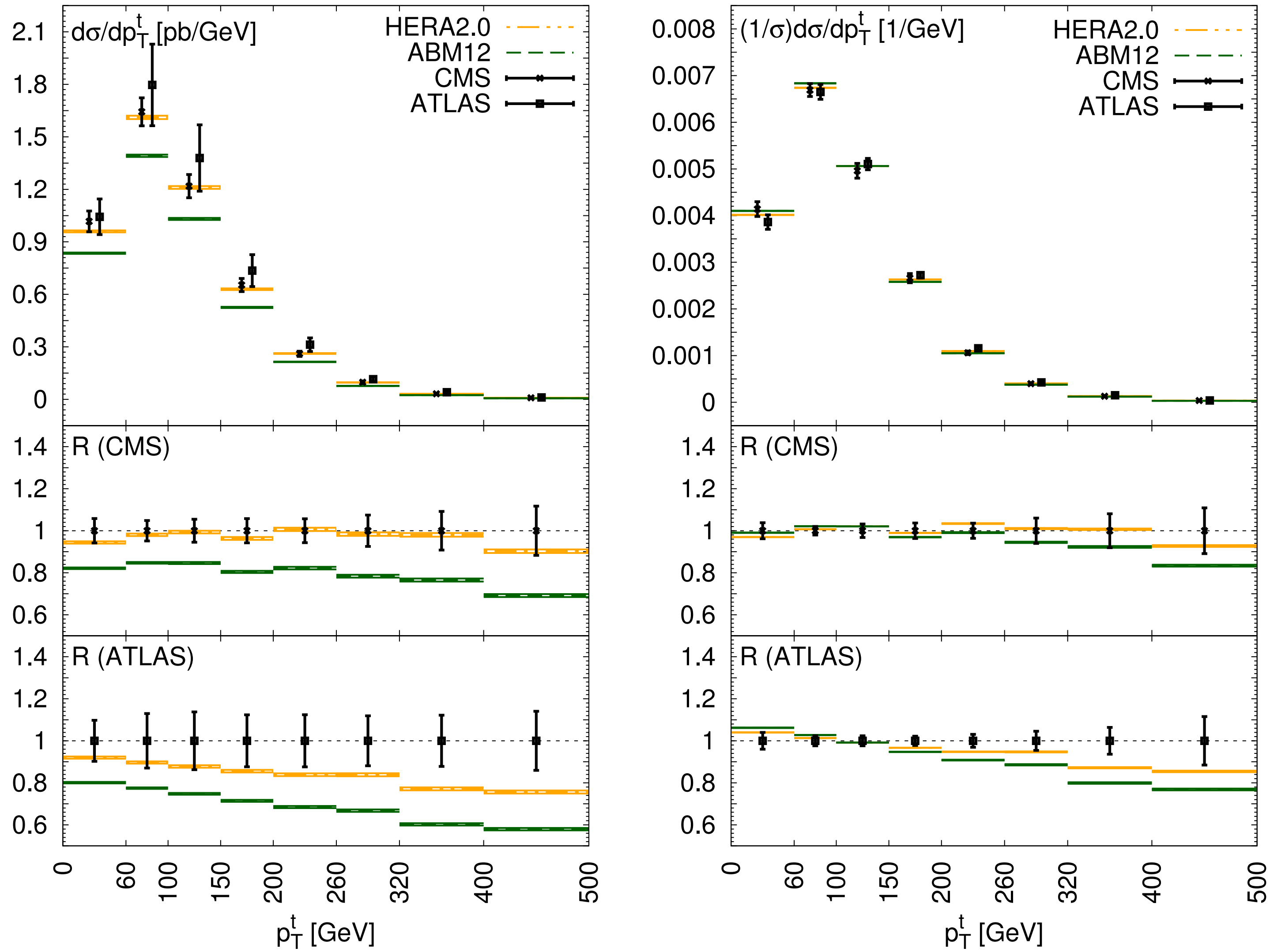


Hartland, Nocera, Rojo, Czakon, Mitov, to appear

Fixing pdf's from existing top data

- Scale variation not included; only pdf error.

ABM12 and HERA2.0: Absolute and Normalized P_T: NNLO



Preliminary

Hartland, Nocera, Rojo, Czakon, Mitov, to appear

Fixing pdf's from existing top data

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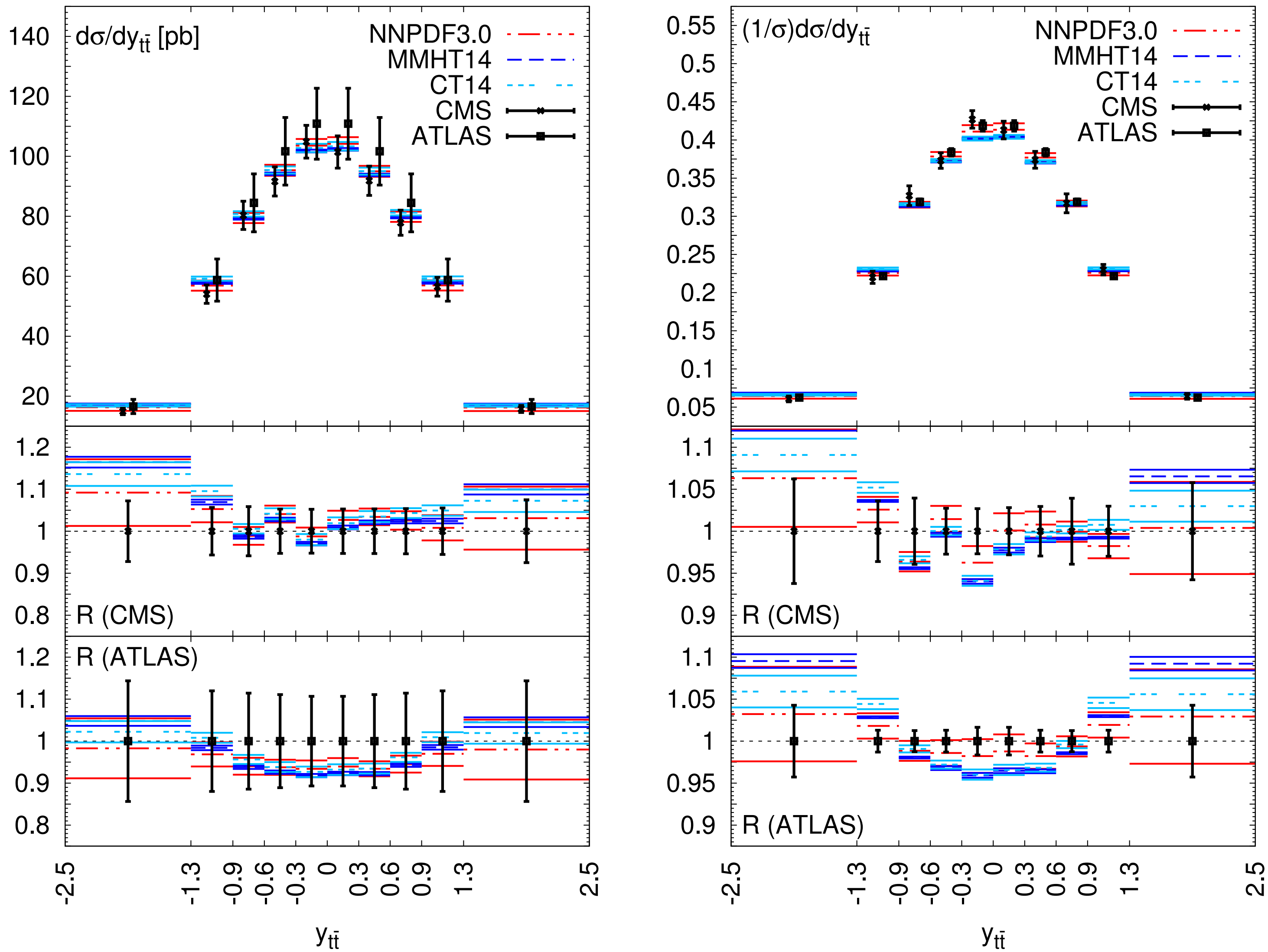
Absolute and Normalized y_{tt}: NNLO

Preliminary

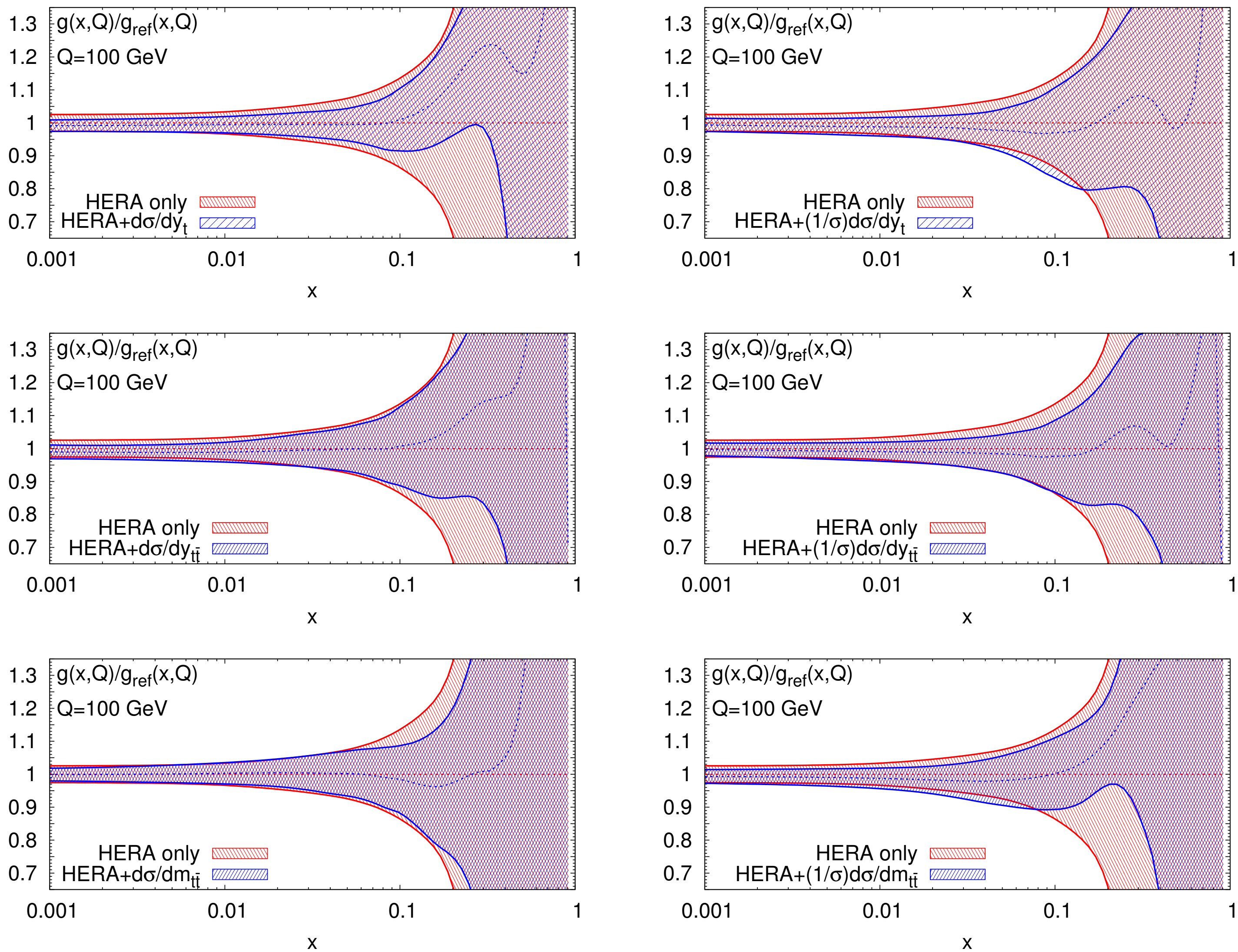


Hartland, Nocera, Rojo, Czakon, Mitov, to appear

Fixing pdf's from existing top data

Gluon PDF before/after inclusion of ATLAS+CMS top data

Preliminary



Hartland, Nocera, Rojo, Czakon, Mitov, to appear

Precision NNLO applications: top mass

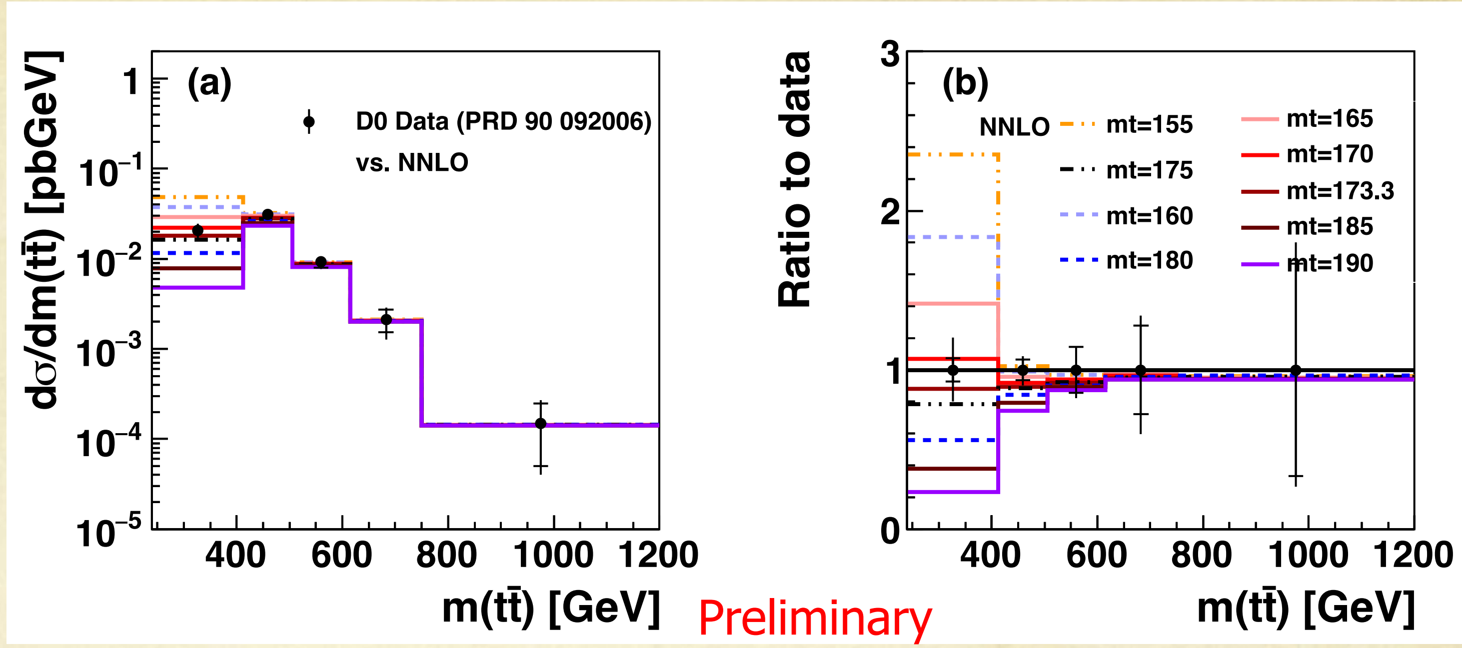
- Another application: top mass from differential distributions at D0

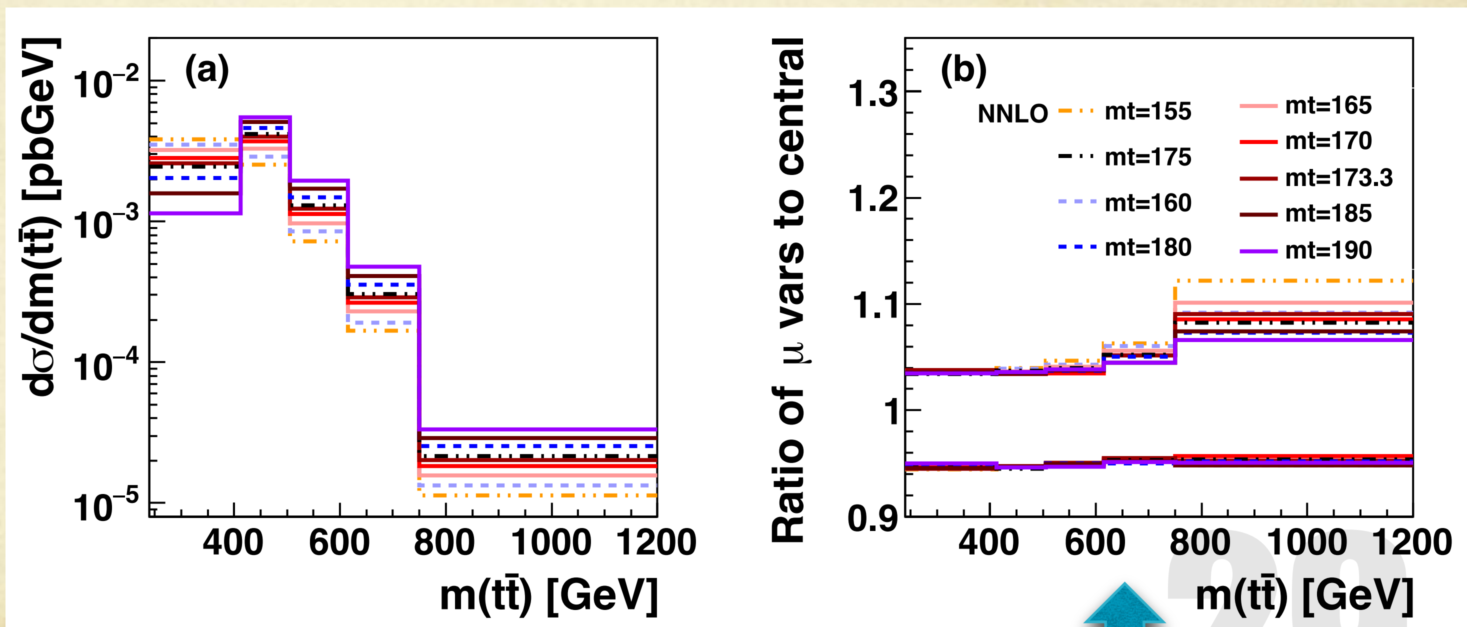
D0 Collaboration + Fiedler, Czakon, Heymes, Mitov, to appear

- Idea:
  - evaluate the main differential distributions for a set of values of m_{top}
  - Consider separately unnormalized and normalized distributions
  - Extract best mass from a chi^2 fit
- The expectation is: extraction should be similar to the D0 one from the total cross-section
- The hope is: the constraining power could be stronger due to correlations through the full spectrum (and not only close to threshold)
- It turns out there is good sensitivity to m_{top} in both un/normalized distributions!
  - This is important because the normalization is strongly dependent on m_{top}
  - (will not show any normalized data – not yet public)
- A good pilot study for the very precise future LHC data!

Precision NNLO applications: top mass

- Unnormalized:
  (m_{top} dependence only
  close to threshold)



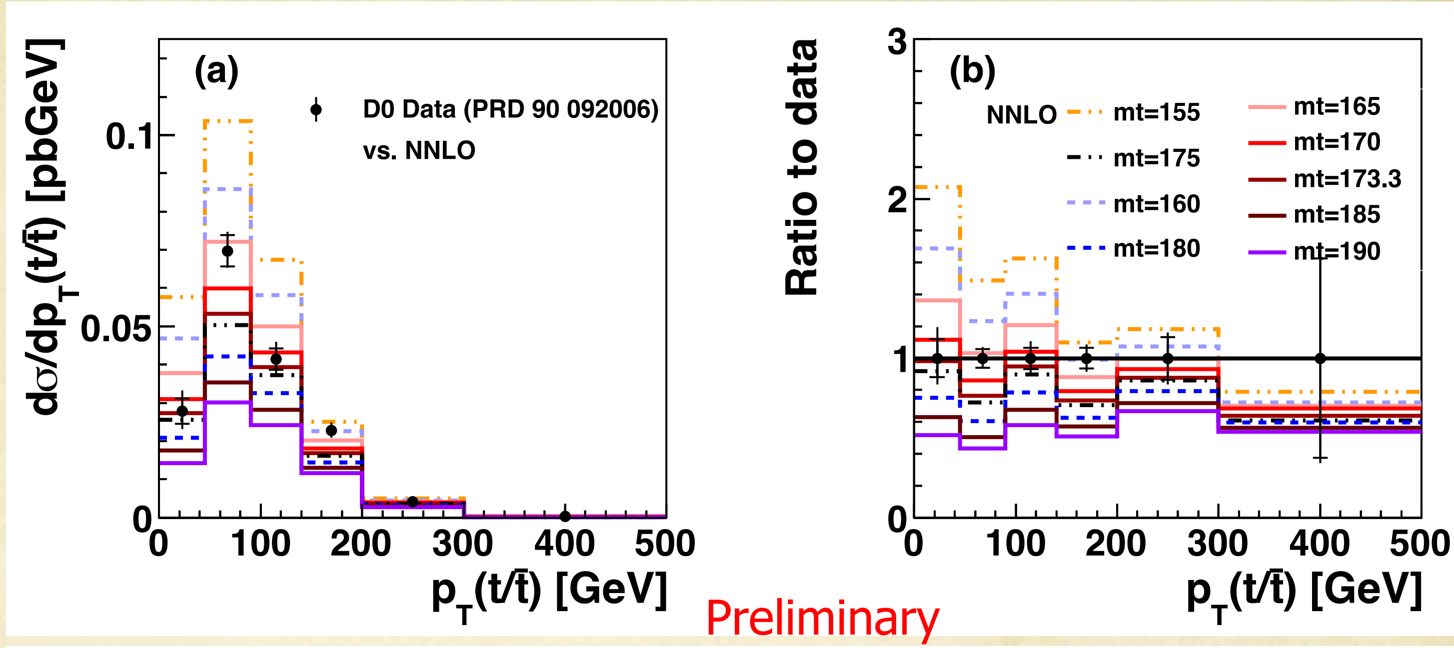


- Normalized:
  (m_{top} dependence
  "reappears" in all bins!)

Relative scale error

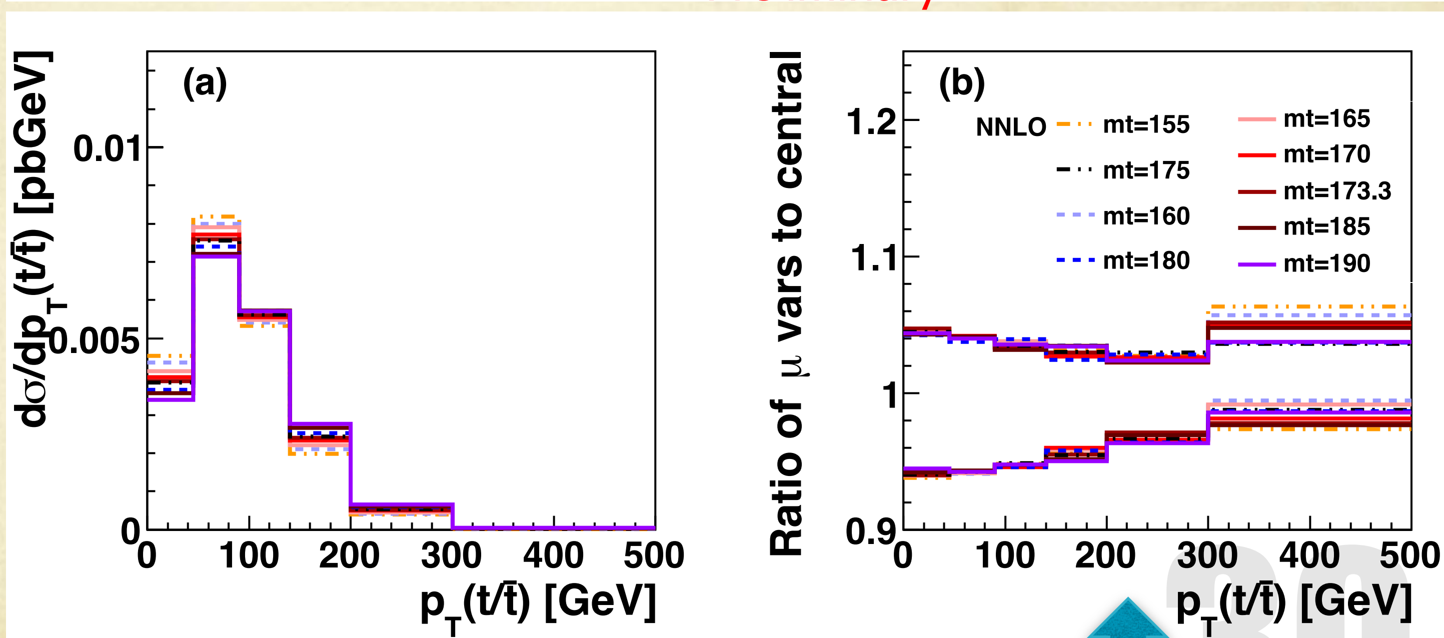
Precision NNLO applications: top mass

- Unnormalized:



Preliminary

- Normalized:



Relative scale error

Conclusions

- Global lessons from NNLO:
  - Precision is generally good (compared to NLO) and makes a difference
  - A large class of processes (2-to-2) has been cleared (only dijets missing)
  - So far this is an incoherent set of calculations
  - To be truly useful we have to take this to the next level
    - Revisit scale choices
    - Ensuring access to calculations and results
    - Fixing pdf's: soon progress will be hampered by the pdf's
- Open issues and future directions:
  - comprehensive NNLO libraries
  - Matching to showers
  - Going to 2-to-3: requires new level of results for 2-loop amplitudes (none exist)