NRQCD approach to $t\bar{t}$ production at threshold

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Plan

Coulomb corrections

- *Top-quark pair production near threshold at LHC*
  Y. Kiyo, J. H. Kühn, S. M., M. Steinhauser and P. Uwer arXiv:0812.0919

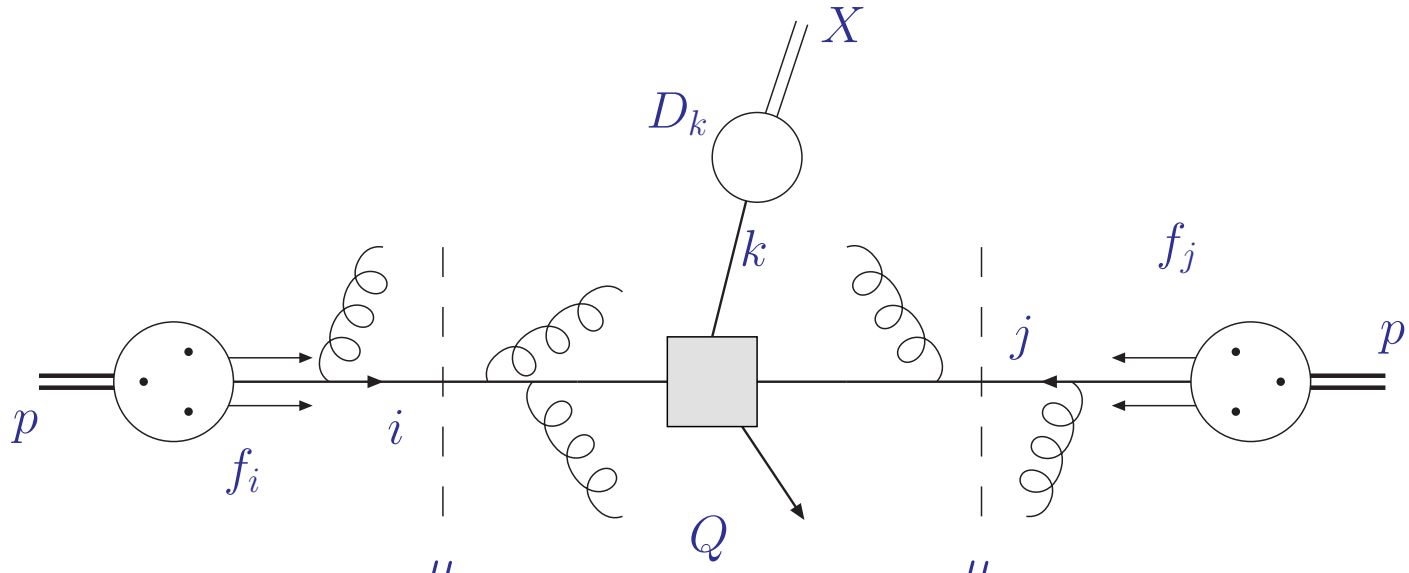
Phenomenology updates

- *Toponium cross section predictions and uncertainty estimates*
  M.V. Garzelli, G. Limatola, S. M., M. Steinhauser and S. Zenaiev
  arXiv:2601.xxxxx

- *Updated predictions for toponium production at the LHC*
  M.V. Garzelli, G. Limatola, S. M., M. Steinhauser and S. Zenaiev
  arXiv:2412.16685

- *Top-quark pole mass extraction at NNLO accuracy, from total, single- and double-differential cross sections for $t\bar{t}+X$ production at the LHC*
  M.V. Garzelli, J. Mazzitelli, S. M. and O. Zenaiev arXiv:2311.05509

QCD factorization



$$\sigma_{pp\to X} = \sum_{ij} f_i(\mu^2) \otimes f_j(\mu^2) \otimes \hat{\sigma}_{ij\to X}\left(\alpha_s(\mu^2), Q^2, \mu^2, m_X^2\right)$$

- Factorization at scale μ
  - separation of sensitivity to dynamics from long and short distances
- Hard parton cross section $\hat{\sigma}_{ij\to X}$ calculable in perturbation theory
  - cross section $\hat{\sigma}_{ij\to k}$ for parton types i, j and hadronic final state X
- Non-perturbative parameters: parton distribution functions f_i, strong coupling α_s, particle masses m_X
  - known from global fits to exp. data, lattice computations, ...

Heavy quark production in perturbation theory

- Cross section for $t\bar{t}$-production

$$\sigma_{pp\to X} = \sum_{ij} f_i(\mu^2) \otimes f_j(\mu^2) \otimes \underbrace{\hat{\sigma}_{ij\to X}\left(\alpha_s(\mu^2), Q^2, \mu^2, m_X^2\right)}$$

$$= \hat{\sigma}^{(0)}_{ij\to X} + \alpha_s\, \hat{\sigma}^{(1)}_{ij\to X} + \alpha_s^2\, \hat{\sigma}^{(2)}_{ij\to X} + \ldots$$

Ingredients

- Hard parton scattering cross section $\hat{\sigma}_{ij\to X}$
  - computed in perturbative QCD
  - NNLO accuracy is state-of-the-art
- Input parameters
  - heavy quark mass in on-shell scheme $m_t^{\rm pole}$
  - strong coupling in $\overline{\rm MS}$-scheme $\alpha_s(M_Z)$
  - proton PDFs f_i

Theory status of fixed order perturbation theory

- NNLO QCD differential predictions for top-quark pairs at the LHC
  Czakon, Heymes, Mitov '15
- Top-quark pair hadroproduction at NNLO in QCD
  Catani, Devoto, Grazzini, Kallweit, Mazzitelli, Sargsyan '19
  - implemented in public release of MATRIX code
    Catani, Devoto, Grazzini, Kallweit, Mazzitelli '19
- NNLO event generation for top-quark pair production (with MiNNLO_PS)
  Mazzitelli, Monni, Nason, Re, Wiesemann and Zanderighi '20; '21
- Narrow-width-approximation at NNLO
  - NNLO QCD corrections to leptonic observables in top-quark pair production and decay
    - implemented in private STRIPPER code
      Czakon, Mitov, Poncelet '20
- Towards NNLO QCD predictions for off-shell top-quark pair production and decays Buonocore, Grazzini, Kallweit, Lindert, Savoini '25

Differential cross sections (I)

Challenges

- NNLO codes not easily publicly usable/accessible
- Very long run times (few CPU years) for distributions with fixed input parameters (m_t, PDFs, . . .)
- Accuracy of NNLO subtraction schemes
  - local sector subtraction (STRIPPER)
  - phase space slicing with $q_T^{\rm cut}$ (MATRIX)

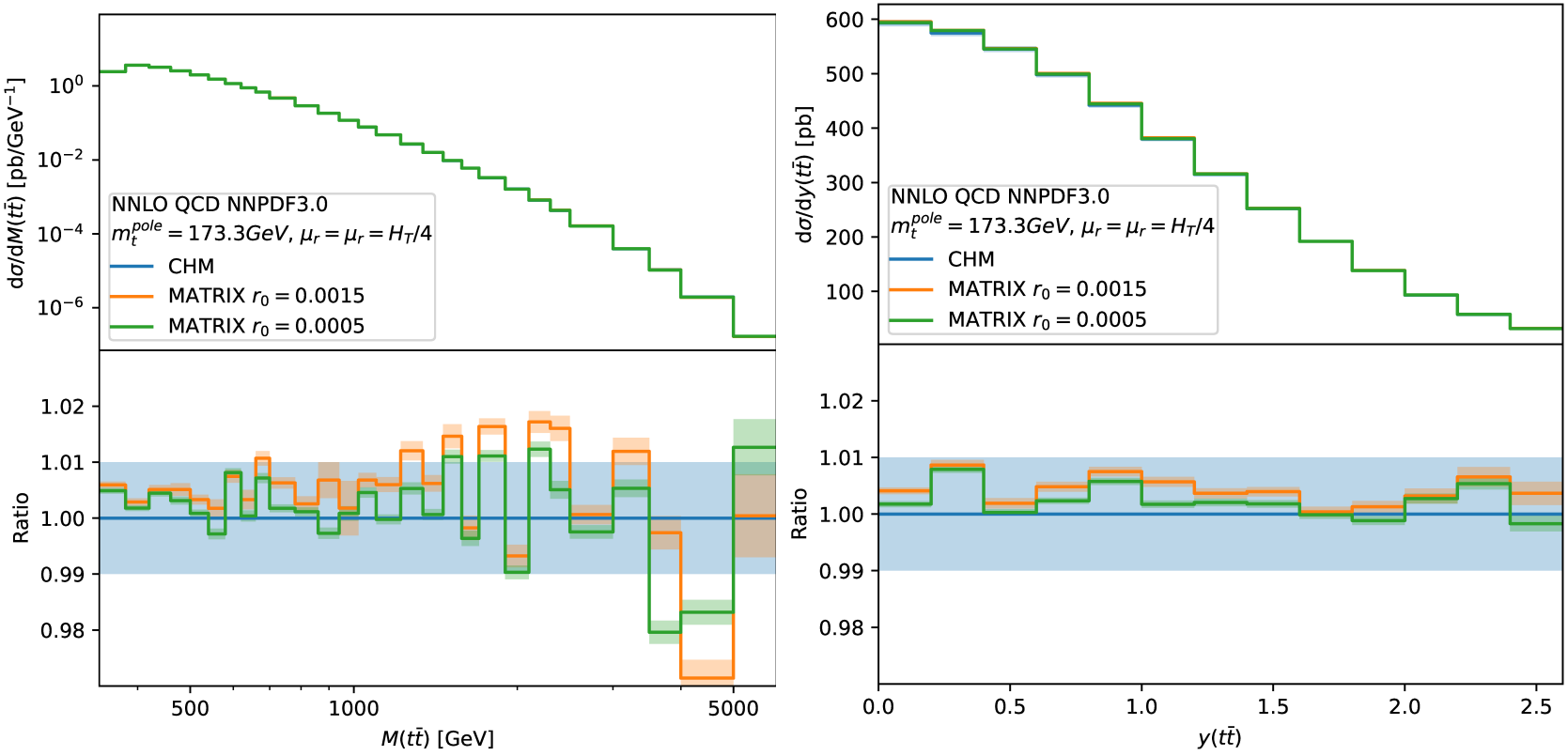
Needs

- NNLO QCD predictions for range of m_t values
- Variation of PDFs (complete set of eigenvectors)

Solution

- Customized version of MATRIX Garzelli, Mazzitelli, SM, Zenaiev '23
  - interface to PineAPPL library for storage of grids
- MATRIX HAWAII (official release) also interfaced to PineAPPL library
  Devoto, Jezo, Kallweit, Schwan '25

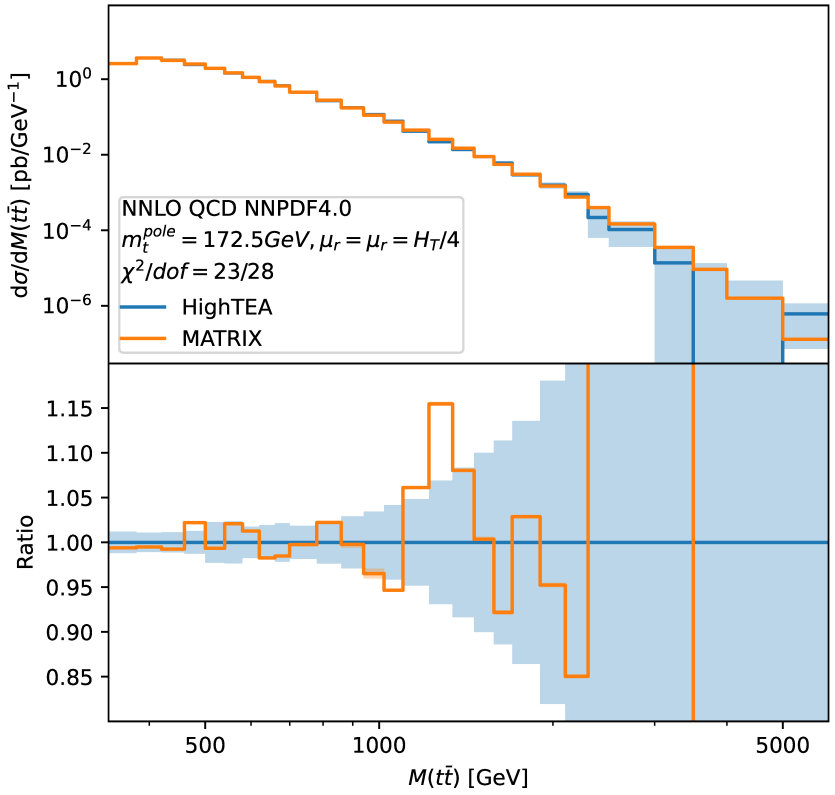
Differential cross sections (II)



- Validation of MATRIX using cuts $r_0 = 0.0015$ and $r_0 = 0.0005$ with results from Czakon, Heymes, Mitov '17 with their numerical uncertainties
- NNLO differential cross sections

  Garzelli, Mazzitelli, SM, Zenaiev '23
  - left: for invariant mass of $t\bar{t}$-pair
  - right: the rapidity of $t\bar{t}$-pair

Differential cross sections (III)



- Validation of MATRIX results for $M(t\bar{t})$ distribution with HighTEA project Czakon, Kassabov, Mitov, Poncelet, Popescu '23.
  - error bars account for numerical uncertainties in computations Garzelli, Mazzitelli, SM, Zenaiev '23

Differential cross sections (IV)

Grids and tables

- PineAPPL grids store genuine NNLO predictions with their exact PDFs, α_s, μ_R, μ_F dependence
  - grids interfaced to PineAPPL library available on
    `https://ploughshare.web.cern.ch/ploughshare/#table1-w`
  - $2 \cdot 10^{11}$ events ($5 \cdot 10^{12}$ weights): 2M CPU hours (3 months real time)
  - numerical uncertainty in bins less than few per mille
- Grids with experimental $t\bar{t} + X$ data available through xFitter project
  `https://gitlab.cern.ch/fitters/xfitter`

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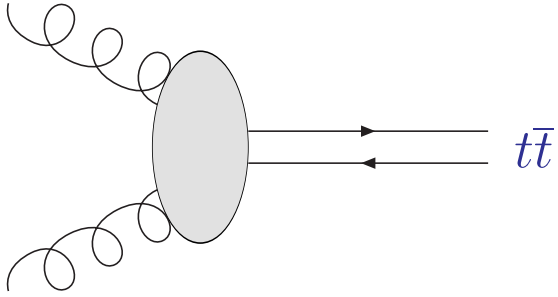
xfitter-cms-ttbar-mt1650-arxiv-2108.02803
xfitter-cms-ttbar-mt1675-arxiv-2108.02803
xfitter-cms-ttbar-mt1700-arxiv-2108.02803
xfitter-cms-ttbar-mt1720-arxiv-2108.02803
xfitter-cms-ttbar-mt1750-arxiv-2108.02803
xfitter-cms-ttbar-mt1775-arxiv-2108.02803
```

  - all grids occupy 6 GB

Heavy quark production near threshold

Quantum numbers

- Quantum numbers of heavy quark pair $t\bar{t}\left({}^{2S+1}L_J^{[1,8]}\right)$
- Notation from spectroscopy
  - orbital angular momentum L:
    $\rightarrow$ S-wave, P-wave, ...
  - spin $2S+1$: singlet, triplet
  - total angular momentum J
  - color $[1,8]$: singlet, octet



Kinematics

- Close to production threshold
  - velocity $\beta_{t\bar{t}} = \sqrt{1-4m^2/s}$ of heavy quarks
- Born cross section near threshold
  - S-wave: $\sigma^{(0)}_{S\text{-wave}} \sim \beta_{t\bar{t}}$
  - P-wave: $\sigma^{(0)}_{P\text{-wave}} \sim \beta^3_{t\bar{t}}$

Cross section (I)

- Parametric form of cross section in $\beta_{t\bar{t}} = \sqrt{1 - 4m^2/s}$

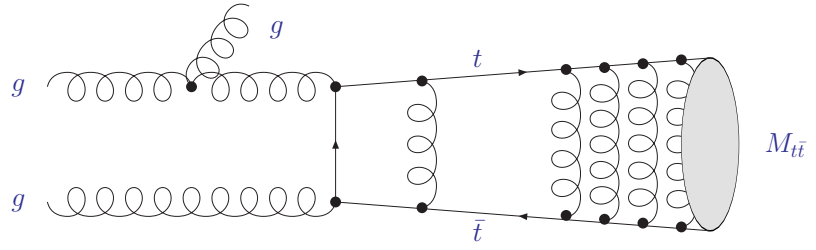
Threshold logarithms

- Sudakov logarithms from emission of soft and collinear gluons
  - all orders in perturbation theory $\alpha_s^n \ln^k(\beta_{t\bar{t}})$ with $2n \geq k \geq 1$
  - resummation of large logarithms (renormalization group equation)

Kidonakis, Sterman '97; Bonciani, Catani, Mangano, Nason '98; ...

Coulomb corrections

- Singular contributions from gluon exchanges among $t\bar{t}$ final state



  - all orders in perturbation theory $\alpha_s^n / \beta_{t\bar{t}}^k$ with $n \geq k \geq 1$
  - resummation with non-relativistic QCD (NRQCD)

Bodwin, Braaten, Lepage '95

Cross section (II)

Perturbation theory

- Partonic cross section

$$\hat{\sigma}_{t\bar{t}} \quad = \quad \hat{\sigma}^{(0)}_{t\bar{t}} \times \sum_{k=0} \left(\frac{\alpha_s}{\beta_{t\bar{t}}} \right)^k \times \exp\Big\{ \underbrace{\ln(\beta_{t\bar{t}}) g_0(\alpha_s \ln(\beta_{t\bar{t}}))}_{\text{LL}} + \underbrace{g_1(\alpha_s \ln(\beta_{t\bar{t}}))}_{\text{NLL}} + \ldots \Big\}$$

- Hadronic cross section
  - convolution with PDFs $\mathcal{L}_{ij} = f_i \otimes f_j$
  - parametric form

$$\frac{d\sigma_{t\bar{t}}}{d\beta_{t\bar{t}}} \quad \simeq \quad \beta_{t\bar{t}}\, \mathcal{L}_{ij}(\beta_{t\bar{t}})\, \hat{\sigma}_{ij\to t\bar{t}}(\beta_{t\bar{t}})$$

- Power counting
  - one power $\beta_{t\bar{t}}$ from Born cross section $\sigma^{(0)}_{S\text{-wave}}$
  - one power $\beta_{t\bar{t}}$ from phase space in convolution with $\mathcal{L}_{ij}$
- Breakdown of fixed order QCD perturbation theory
  - $d\sigma^{\text{LO}}_{t\bar{t}} \sim \beta^2_{t\bar{t}}$, $\ldots$, $d\sigma^{\text{N}^3\text{LO}}_{t\bar{t}} \sim \frac{1}{\beta_{t\bar{t}}}$, $d\sigma^{\text{N}^4\text{LO}}_{t\bar{t}} \sim \frac{1}{\beta^2_{t\bar{t}}}$, $\ldots$

Phenomenology

- **FCC-ee**: much work (theory and phenomenology) [many people]
  - fixed center-of-mass energy S allows $t\bar{t}$ threshold scan at $\sqrt{S} \sim 2m_t$
  - dominant color-singlet production $\to t\bar{t}\left({}^3S_1^{[1]}\right)$
- **FCC-ee**: bound state corrections also for other charged final states
  - W^+W^--pairs with corrections from Coulomb photons
    $\Delta\sigma/\sigma_{\text{Born}} \simeq \mathcal{O}(\text{few})$ ‰ Fadin, Khoze, Martin, Stirling '95, Fadin, Khoze, Martin, Chapovsky '95, Actis, Beneke, Falgari, Schwinn '08
- **LHC**: effects on top-mass measurement Hagiwara, Sumino, Yokoya '08
  - dominant color-singlet production $\to t\bar{t}\left({}^1S_0^{[1]}\right)$
  - complete NLO NRQCD result Petrelli, Cacciari, Greco, Maltoni, Mangano '97 (corrections by Hagiwara, Sumino, Yokoya '08)
  - detailed study in NRQCD assembling existing knowledge at NLO/NLL Kiyo, Kühn, S.M., Steinhauser, Uwer '08
  - bound-state effects on kinematical distributions Sumino, Yokoya '10
  - more studies since 2020 ...

Theory framework for hadro-production

- Recall master equation $\sigma_{pp\to t\bar{t}} = \sum_{ij} f_i \otimes f_j \otimes \hat{\sigma}_{ij\to t\bar{t}}$
  - top-quark pairs produced as color-singlet/octet $\to t\bar{t}\left({}^{2s+1}S_J^{[1,8]}\right)$
  - threshold at $M_{t\bar{t}} \sim 2m_t$ with $M_{t\bar{t}} = (p_t + p_{\bar{t}})^2$

NRQCD factorization

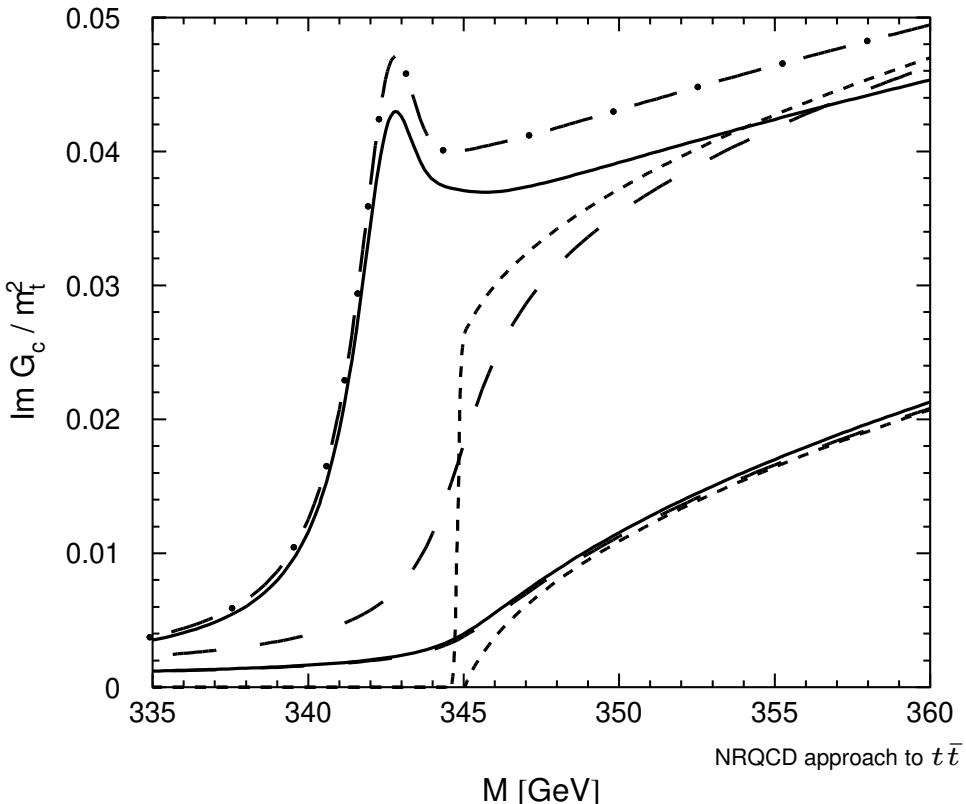
- Partonic cross section $\hat{\sigma}_{ij\to t\bar{t}} = F_{ij\to T} \times \Im G(M_{t\bar{t}})$
  - free $t\bar{t}$ production rate $F_{ij\to T}$
  - "bound state" Green's function $\Im G$ (imaginary part)
- Coulomb resummation from solution of Schrödinger equation in NRQCD with QCD heavy quark potential $V_{\text{QCD}}^{[1,8]}(\vec{x})$
  - small energies $E = E_t + E_{\bar{t}} - 2m_t$ in toponium rest frame

$$\left\{-\frac{\vec{\nabla}^2}{m_t} + V_{\text{QCD}}^{[1,8]}(\vec{x}) - (E + \mathrm{i}\Gamma_t)\right\} G^{[1,8]}(E,\vec{x}) \quad = \quad \delta^{(3)}(\vec{x})$$

- Differential kinematics $\dfrac{d\hat{\sigma}_{ij\to t\bar{t}}}{dM_{t\bar{t}}^2} = F_{ij\to T} \times \Im G^{[1,8]}(M_{t\bar{t}})$
  - soft-collinear resummation in $F_{ij\to T}$ at NLL and matching at NLO

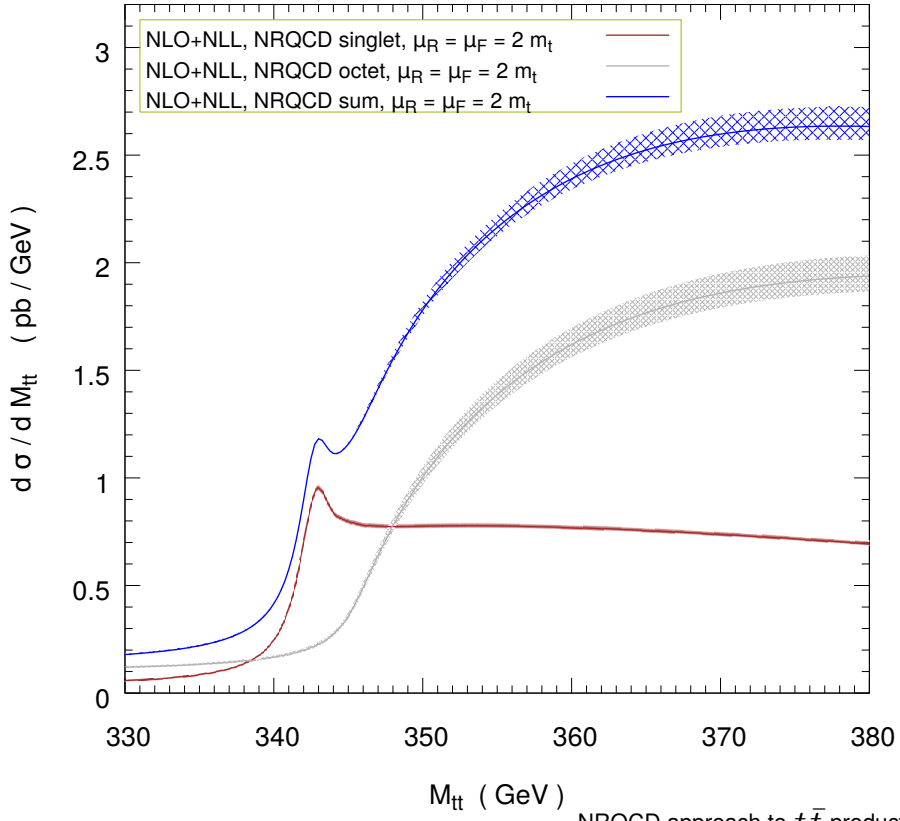
Green's function

- Green's function $\Im G$ (imaginary part)
  - NLO color singlet $\Im G^{[1]}$ (upper solid line)
  - NLO color octet $\Im G^{[8]}$ (lower solid line)
  - NNLO contribution of $V_{\rm QCD}^{[1]}(\vec{x})$ to color singlet $\Im G^{[1]}$ (dash-dotted line)
  - expansions of $\Im G^{[1]}$ in fixed order up to $\mathcal{O}(\alpha_s)$ with (dashed) and without Γ_t (dotted line)



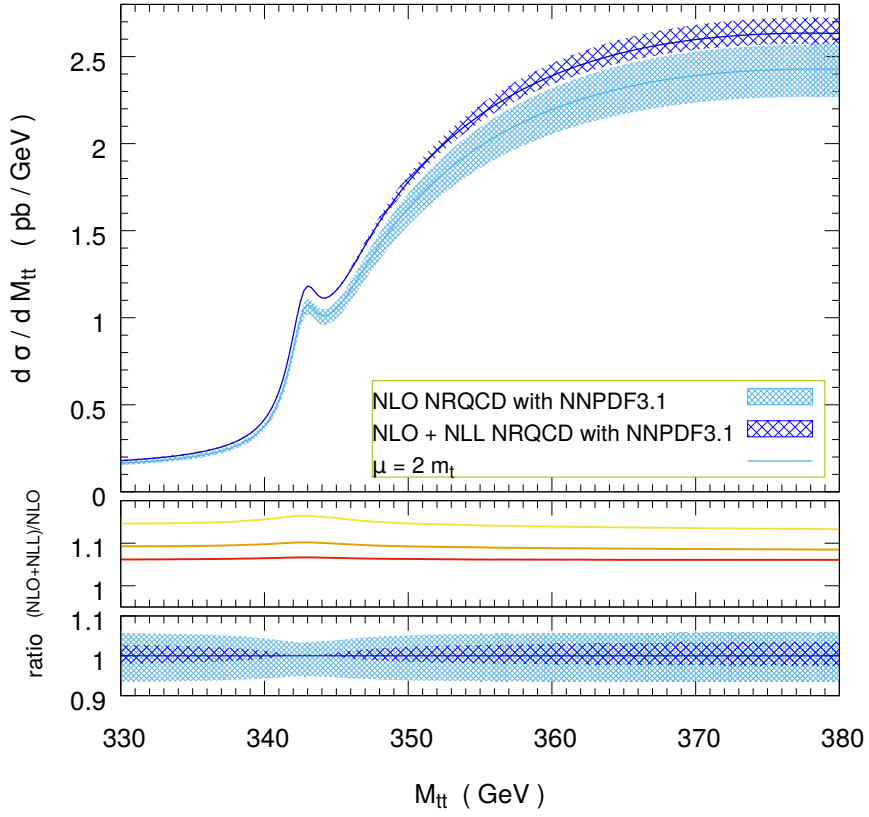
Invariant mass distristribution (I)

- $d\sigma/dM_{t\bar{t}}$ at LHC ($\sqrt{S} = 13$ TeV) Garzelli, Limatola, S.M., Steinhauser, Zenaiev '24
- Parton channels with large threshold logarithms
  - $gg \to t\bar{t}\left({}^1S_0^{[1]}\right)$ attractive interaction $\to$ Coulomb resonance
  - $gg \to t\bar{t}\left({}^1S_0^{[8]}\right)$, $q\bar{q} \to t\bar{t}\left({}^3S_1^{[8]}\right)$ repulsive interaction



Invariant mass distristribution (II)

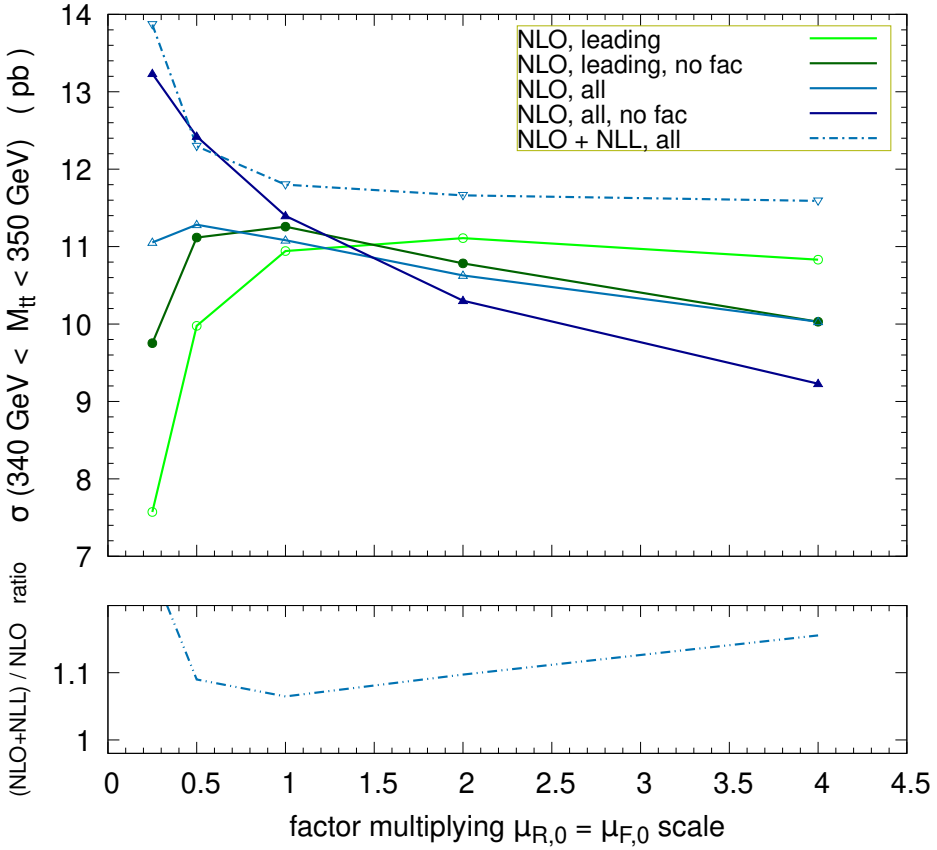
- $d\sigma/dM_{t\bar{t}}$ at LHC ($\sqrt{S} = 13$ TeV) for top quark pole mass $m_t = 172.5$ GeV
  - fixed order NLO vs. NLO+NLL resummed NRQCD predictions
  - scale variation $\mu_r = \mu_f \in \{m_t, 2m_t, 4m_t\}$



- S-wave channels without large threshold logs (omitted in resummation)
  - $gg \to {}^3S_1^{[1,8]}$, $q\bar{q} \to {}^1S_0^{[1,8]}$, $gq \to {}^1S_0^{[1,8]}$, $gq \to {}^3S_1^{[8]}$ sum up to $\mathcal{O}(5\%)$

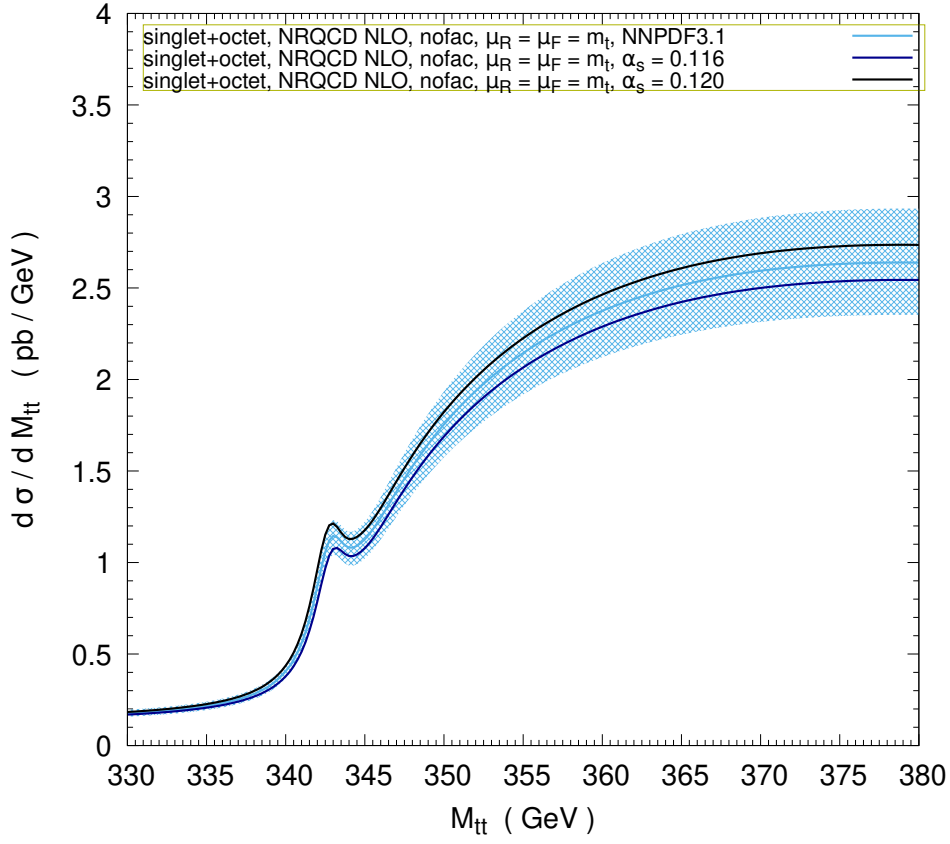
Uncertainties: scales

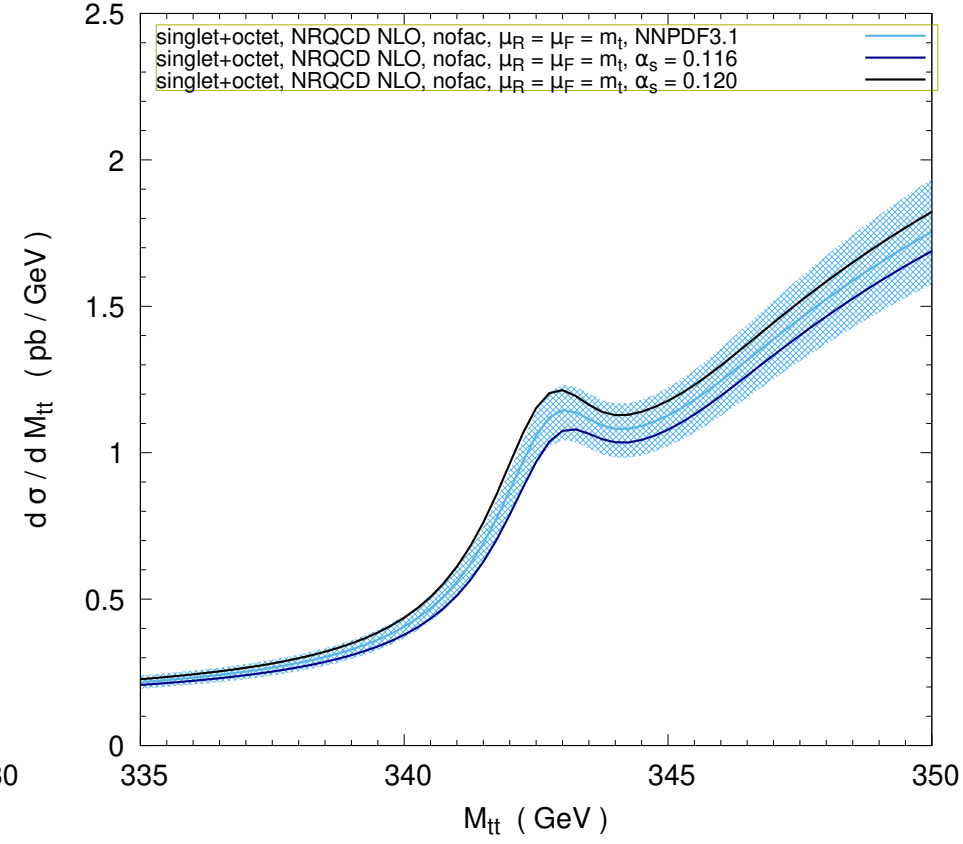
- $d\sigma/dM_{t\bar{t}}$ with NNPDF3.1 PDFs; threshold at $dM_{t\bar{t}} = 345$ GeV
  - bin 340 GeV $< M_{t\bar{t}} < 350$ GeV
- NLO NRQCD predictions with μ_R, μ_F variation
  - minimal sensitivity at $\mu_R \simeq \mu_F \simeq m_t$
    (also supported by NLL resummation)



Uncertainties: strong coupling

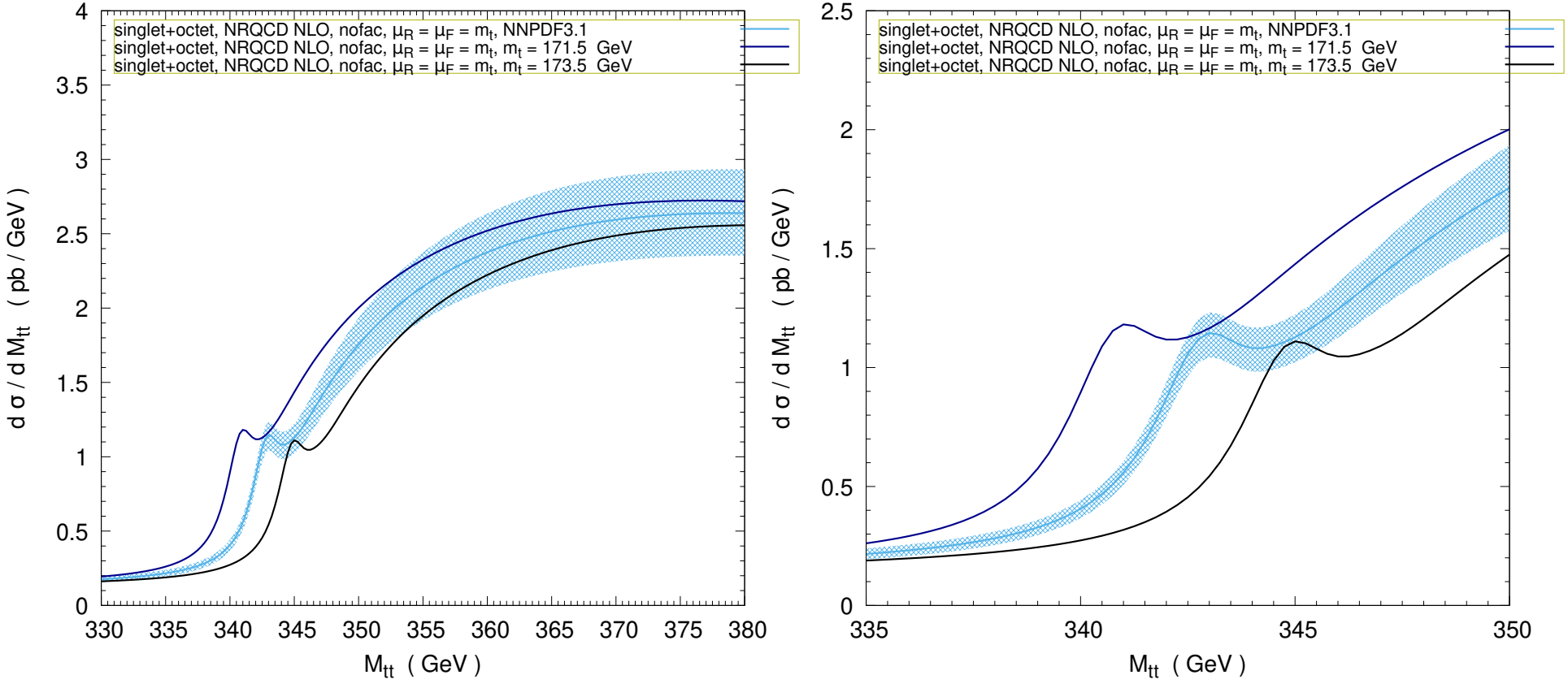
- NLO NRQCD predictions for $d\sigma/dM_{t\bar{t}}$ with NNPDF3.1 PDFs
- variation of strong coupling $\alpha_s(M_Z)$
  - cross section directly proportional to value of $\alpha_s(M_Z)$





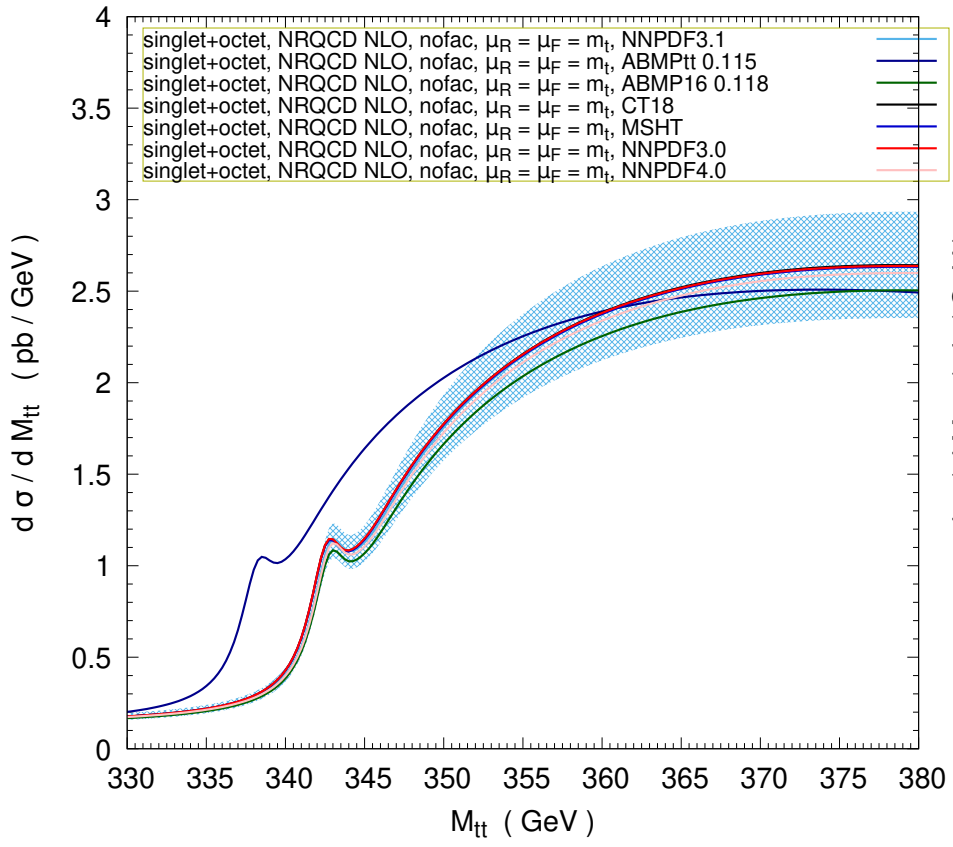
Uncertainties: top-quark mass

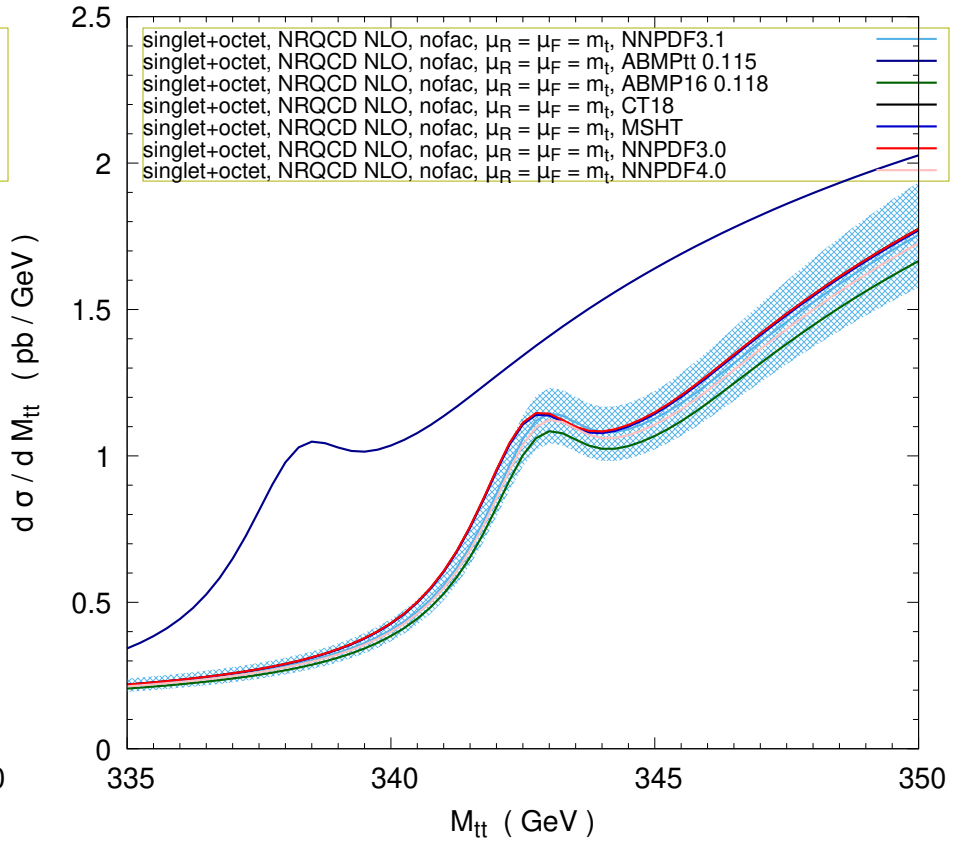
- NLO NRQCD predictions for $d\sigma/dM_{t\bar{t}}$ with NNPDF3.1 PDFs
- top-quark mass values 171.5 GeV,$\ldots,173.5$ GeV
  - shift of threshold as function of m_t



Uncertainties: PDFs

- NLO NRQCD predictions for $d\sigma/dM_{t\bar{t}}$
- PDF variation
  - all PDFs (except ABMPtt) with $m_t = 172.5$ GeV and $\alpha_s(M_Z) = 0.1180$
  - ABMPtt PDFs with $m_t = 170.3$ GeV and $\alpha_s(M_Z) = 0.1150$



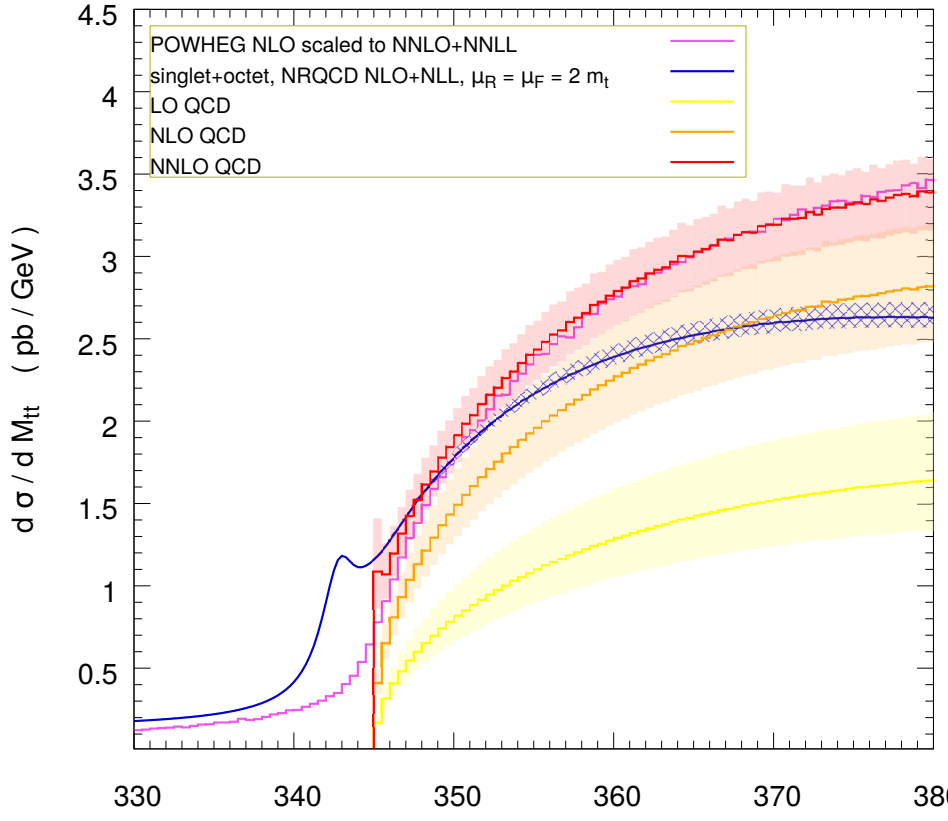


Matching to fixed order (I)

- $d\sigma/dM_{t\bar{t}}$ with NNPDF3.1 PDFs; threshold at $dM_{t\bar{t}} = 345$ GeV
  - NLO+NLL resummed NRQCD predictions
  - fixed order QCD at LO, NLO, NNLO with adapted version of MATRIX

    Garzelli, Mazzitelli, S.M., Zenaiev '23
  - POWHEG (rescaled to NNLO+NNLL total cross section)

    Anuar, Grohsjean, Jeppe, Schwanenberger [private work]

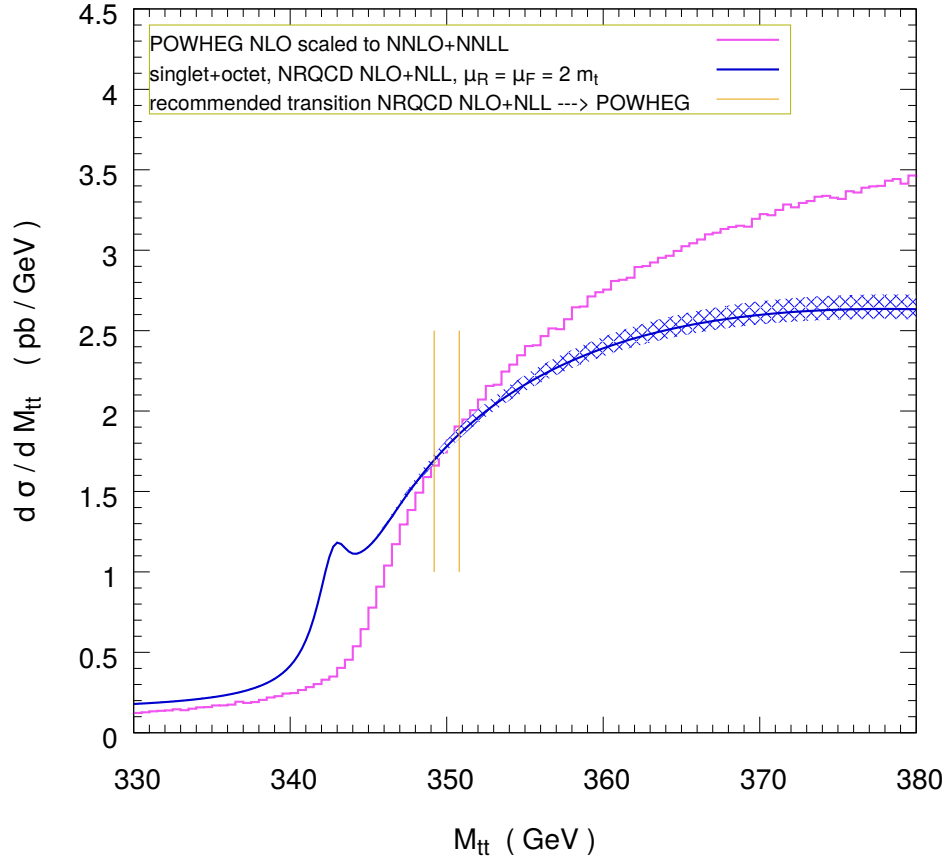


Matching to fixed order (II)

- $d\sigma/dM_{t\bar{t}}$ with matching of NRQCD to fixed order perturbation theory
  - NLO+NLL resummed NRQCD predictions
  - NLO+POWHEG (rescaled to NNLO+NNLL total cross section)

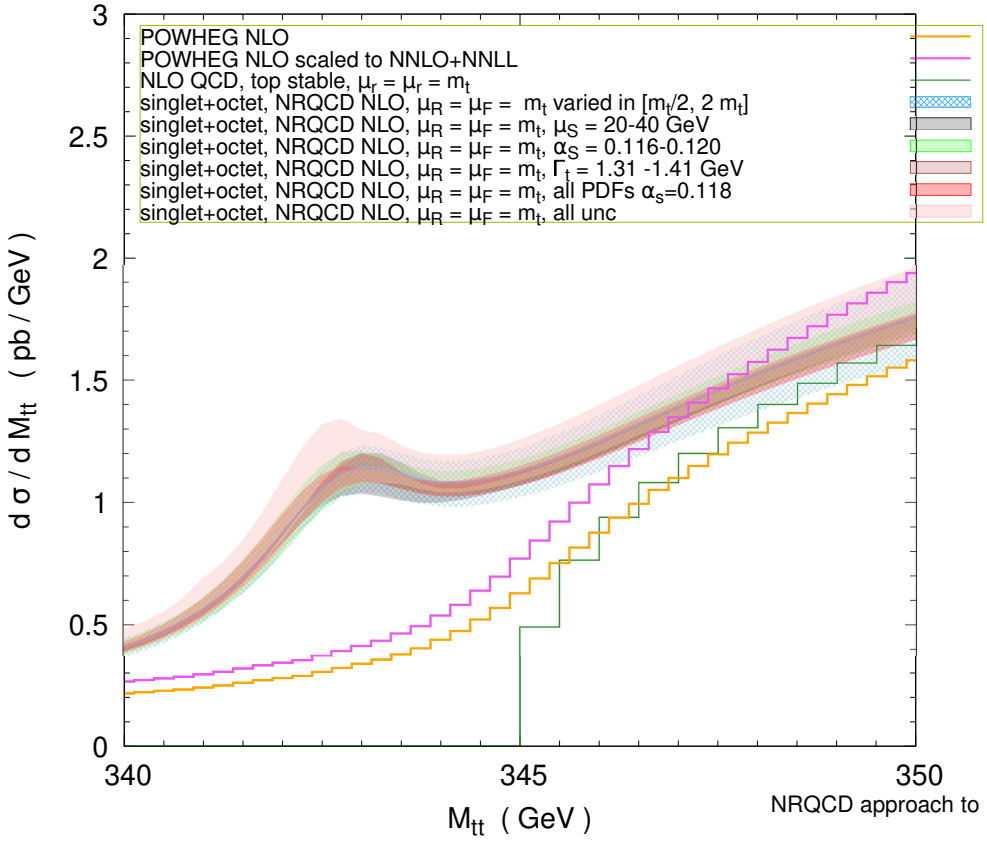
Anuar, Grohsjean, Jeppe, Schwanenberger [private work]

- Validity of NRQCD theory framework in range $M_{t\bar{t}} \in [340, 350]$ GeV



Toponium cross section

- $d\sigma/dM_{t\bar{t}}$ in bin $340\ \text{GeV} < M_{t\bar{t}} < 350\ \text{GeV}$ at $\mu_R = \mu_F = m_t$
  - NLO NRQCD $\sigma = 11.94 + 1.56 - 1.58$ pb
  - NLO+NLL NRQCD $\sigma = 12.36 + 1.22 - 1.08$ pb
- Determination of excess cross section $\Delta\sigma$ as observed by ATLAS, CMS dependent on bin size, order of perturbation theory, rescaling etc.
  - fixed order NLO with stable $t\bar{t}$ leads to $\Delta\sigma \simeq \mathcal{O}(6-7)$ pb



Summary

Status

- Coulomb corrections and their resummation for $t\bar{t} + X$ production
  - update of resummation studies at NLL for ATLAS, CMS analyses
  - comprehensive uncertainty estimates
- Determination of toponium cross section (bin $340\ \text{GeV} < M_{t\bar{t}} < 350\ \text{GeV}$)
- Combination with QCD perturbation theory to NNLO for $t\bar{t} + X$ production
  - bin-wise matching

Outlook

- Dedicated matching computation for NRQCD and fixed-order QCD perturbation theory
  - procedure for experimental analyses
- Theory improvements
  - Coulomb corrections for $t\bar{t} + X$ hadro-production at NNLO
  - Threshold resummation at NNLL