Theory predictions and Monte Carlo modeling for top quark physics

“Some highlights since the Freiburg SM@LHC conference”.

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Theory predictions and Monte Carlo modeling for top quark physics

[SM@LHC 2014 Conference – CIEMAT Madrid]

Jan Winter

– MPP Munich, Germany –

Max-Planck-Institut für Physik
(Werner-Heisenberg-Institut)

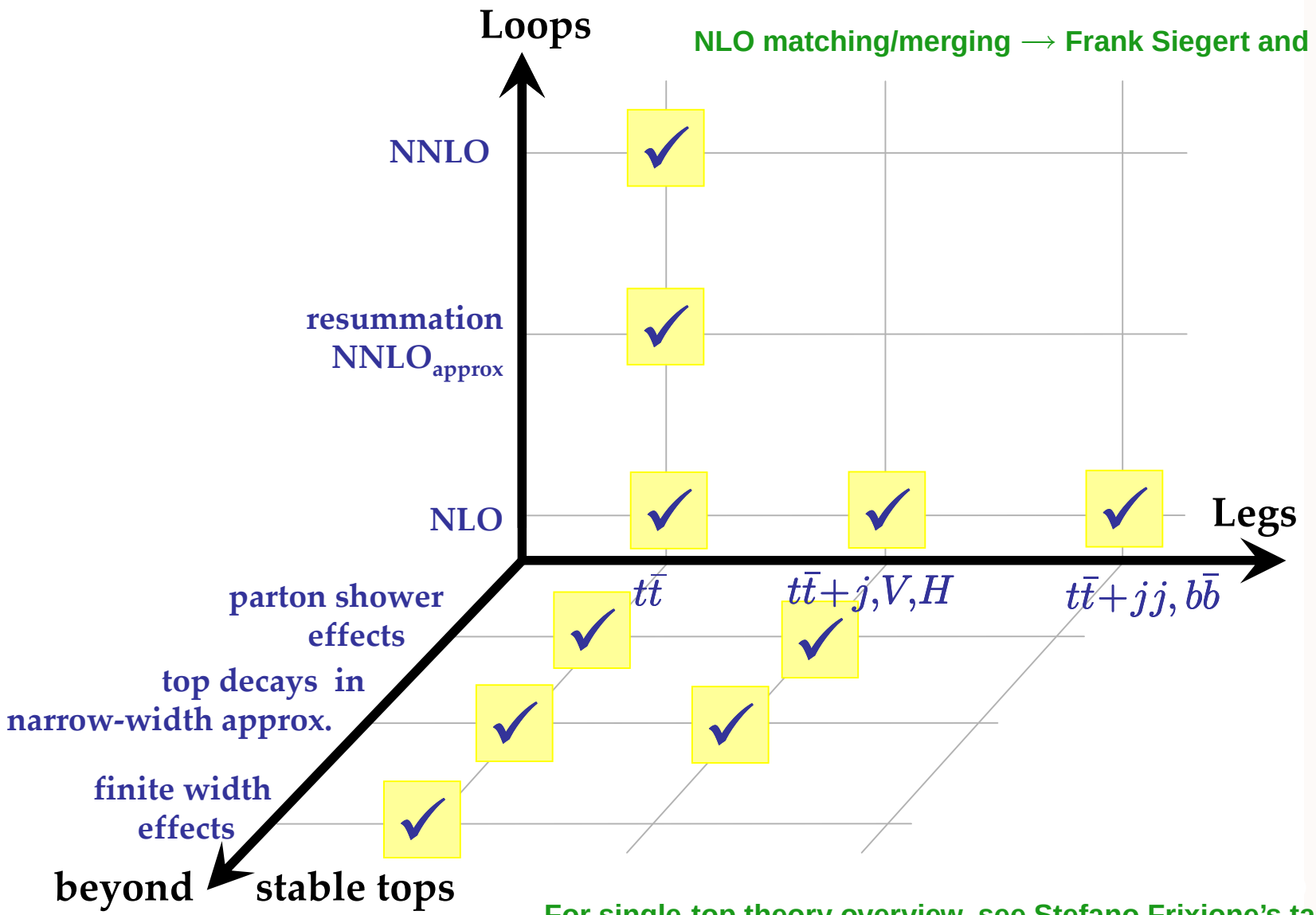
➡ *Will briefly discuss:*

- *Selected new achievements in $t\bar{t} + X$ calculations.*
- *Top quark asymmetries and higher orders.*
- *Top quark mass determination and scale uncertainties.*
- *Summary & Outlook.*

Overview of talk

➡ *Directions in theory space – help "locate" new developments.*

[COURTESY OF MARKUS SCHULZE]



NLO matching/merging ⟶ Frank Siegert and Stefan Prestel's talks.

For single-top theory overview, see Stefano Frixione's talk tomorrow morning.

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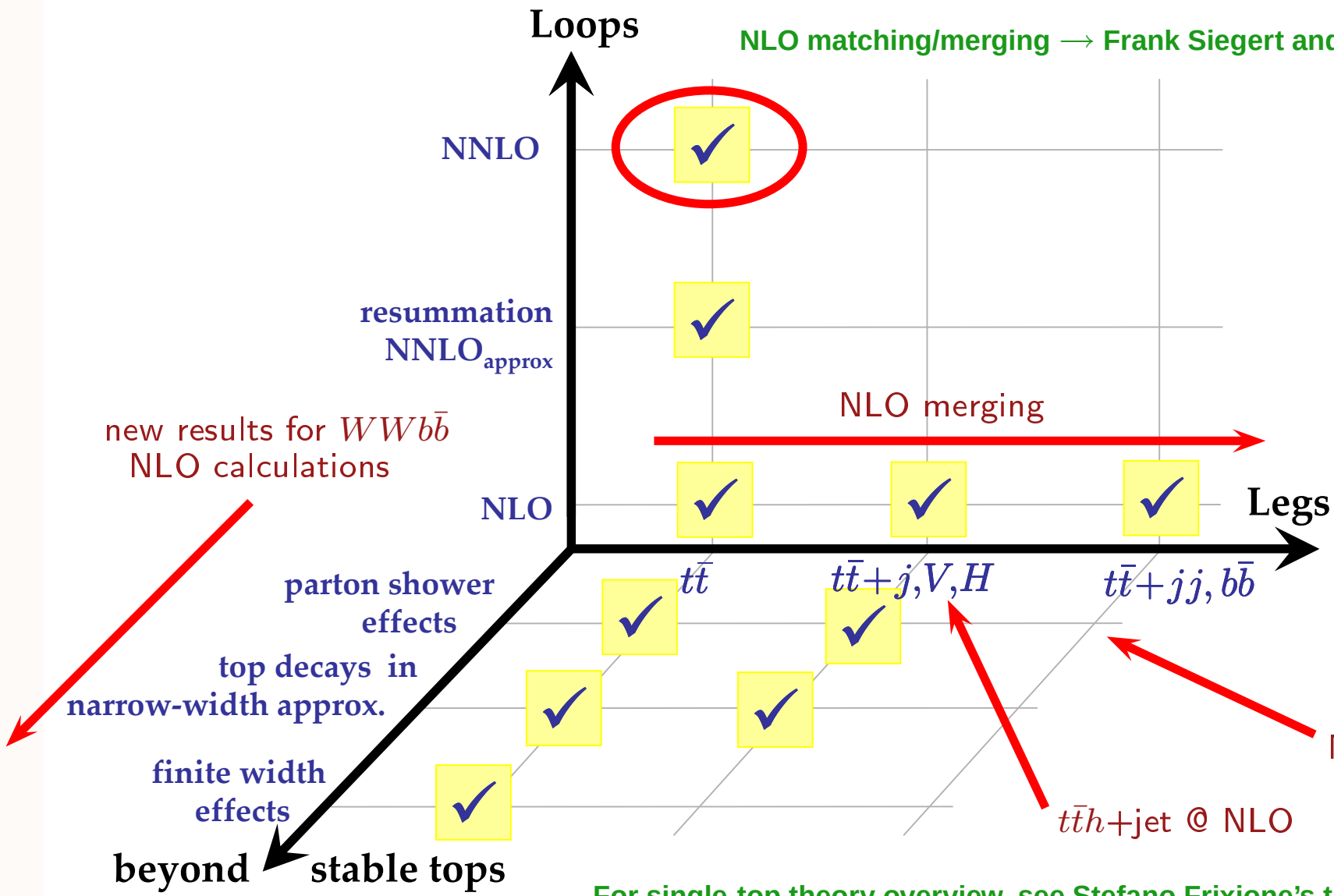

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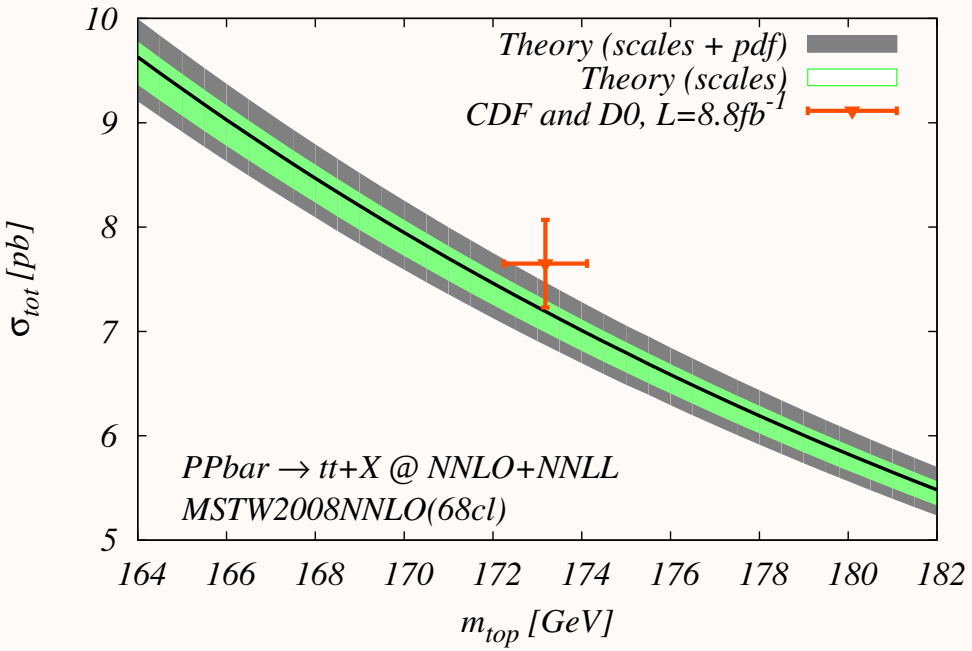
Precision calculation frontier

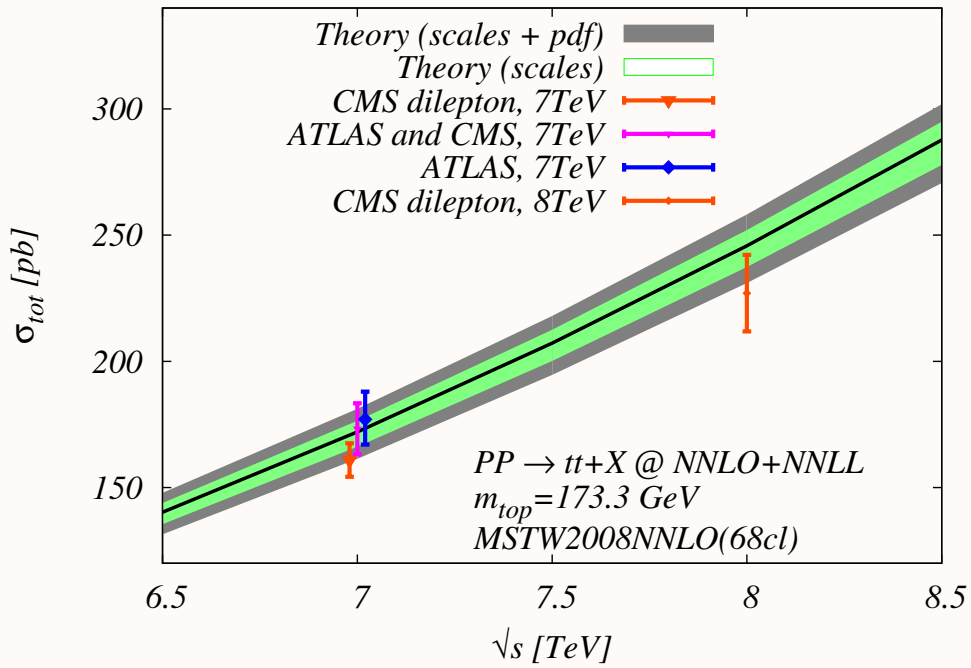
[Czakon, Fiedler, Mitov, arXiv:1303.6254]

just completed last year, NNLO+NNLL cross section for top quark pair production

(left) predicted xsec at the Tevatron as a function of the top quark mass, compared to a recent combination of Tevatron measurements.

(right) predicted xsec at the LHC as a function of the collider c.m. energy, compared to available ATLAS and/or CMS measurements.





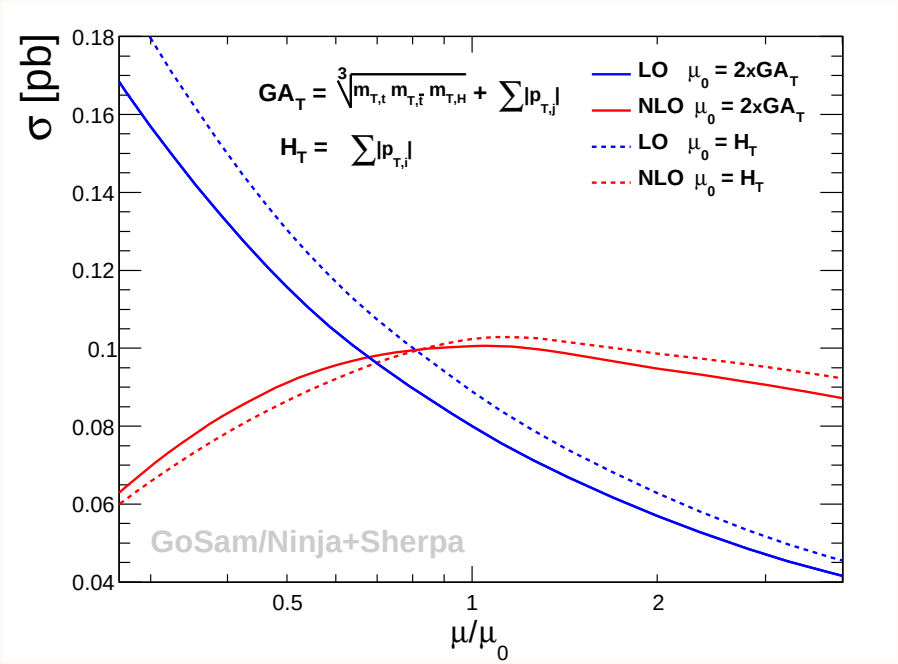
➡ Build parton-level event generator next to give access to differential distributions.

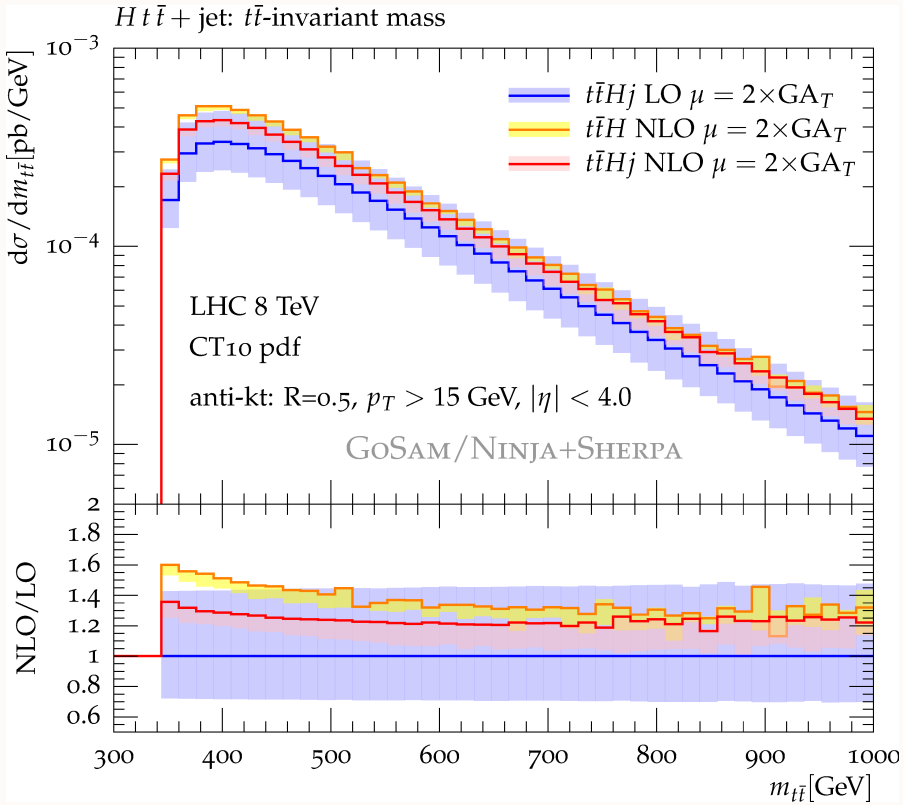
$t\bar{t}h$+jet production at NLO

➡ ***Calculated with GoSam/Ninja+Sherpa combined MC package.***

- $t\bar{t}h$+jets relevant for determination of Higgs-top Yukawa coupling
- interesting case (also from computational point of view) since several mass scales are involved; m_h, m_t
- two different scale choices that give very similar cross section results (left)

[VAN DEURZEN, LUISONI ET AL. ARXIV:1307.8437]





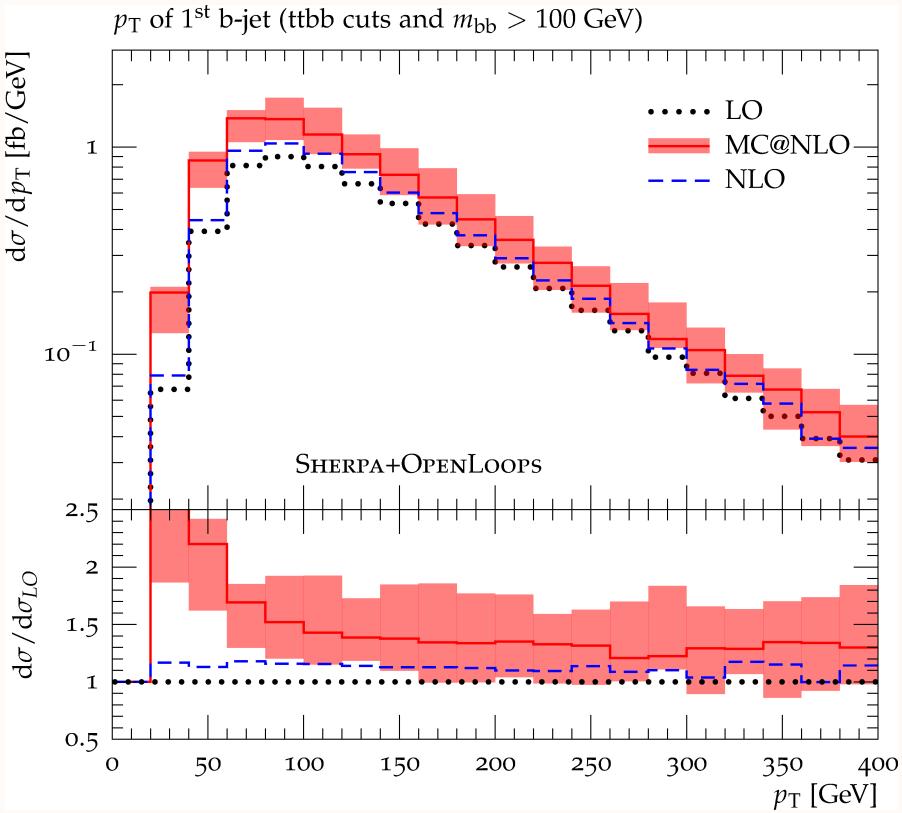
- (right) invariant mass of top quark pair, showing significant impact of NLO corrections

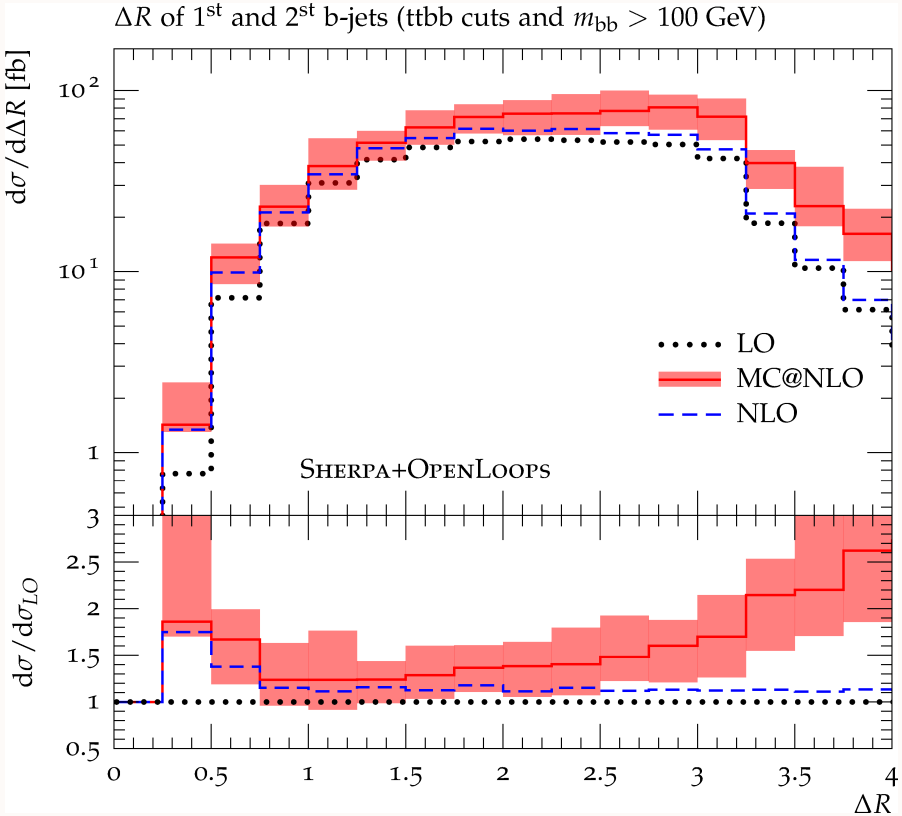
NLO matched $t\bar{t}\,b\bar{b}$ with massive b-quarks

➡ ***Calculated with OpenLoops + Collier + Sherpa.***

[Cascioli, Maierhöfer, Moretti, Pozzorini, Siegert, arXiv:1309.5912]
see also [Kardos, Trocsanyi, arXiv:1303.6291]

- important background to $ht\bar{t}$ signal
- first complete MC@NLO simulation of this process including b-quark mass effects
- NLO predictions for arbitrary $t\bar{t}b\bar{b}$ kinematics, e.g. one or both b-jets from collinear gluon splittings





- b-jet is any jet containing at least a b-quark; $m_{bb} > 100$ GeV to project $t\bar{t}h$ signal region, contaminated by sizeable MC@NLO enhancements due to double collinear $g \to b\bar{b}$ splittings

Monte Carlo event generation

Event generators are used to model multi-hadron final states of high-energy particle collisions.

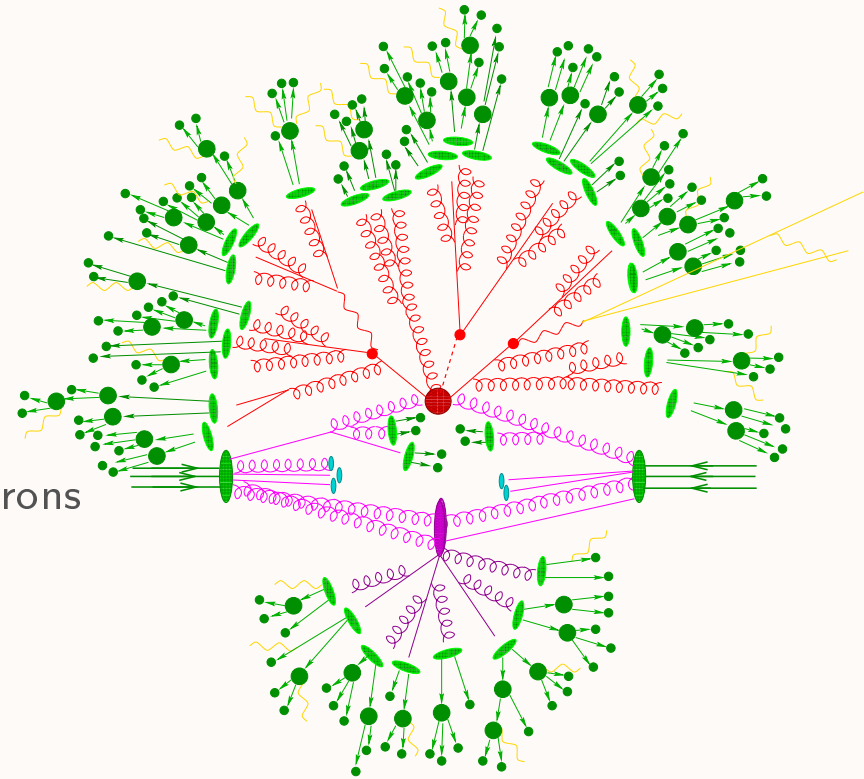
Factorization approach: divide jet simulation into different phases – use Monte Carlo methods.

➡ ***Perturbative Phases:*** *[parton jets]*

- ***Hard process/interaction (hard jet production)***
  exact matrix elements $|\mathcal{M}|^2$ ***[ME]***
- ***QCD bremsstrahlung (soft/coll multiple emissions)***
  initial- and final-state parton showering ***[PS]***

- ***Multiple/Secondary interactions***
  modelling the underlying event

⇐ current frontier is ME+PS matching at NLO+(∼N)LL and merging different jet bins with no double counting



➡ ***Non-perturbative Phases:*** *[jet confinement – particle jets]*

- ***Hadronization***
  phenomenological models to convert partons into primary hadrons
- ***Hadron decays***
  phase-space or effective models to decay unstable into stable hadrons as observed in detectors

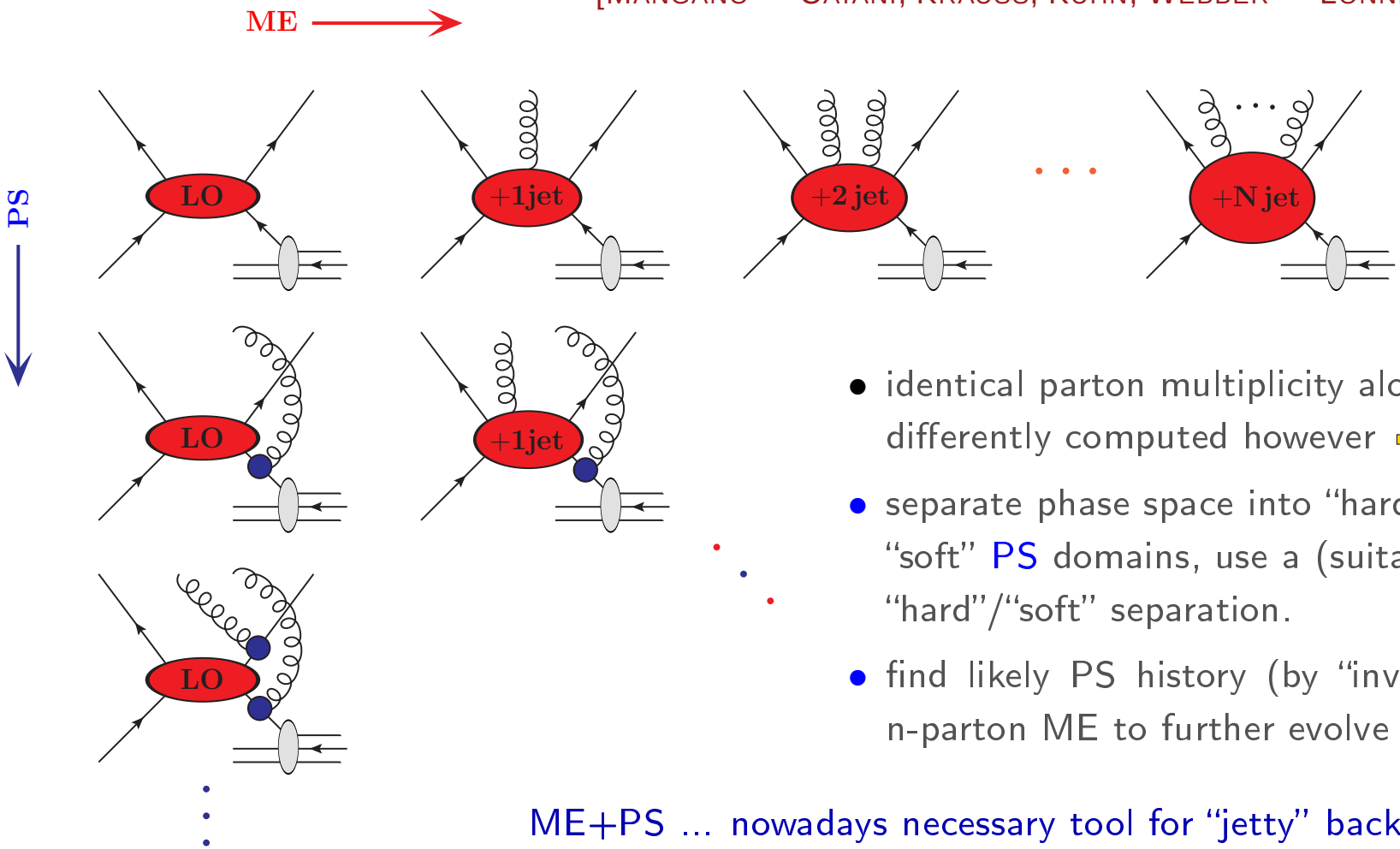
Matrix-element + parton-shower merging (ME+PS)

➡ combine PS pros (resumming soft emissions) + ME pros (hard emissions, quantum interferences, correlations)

⇒ Fully populate emission's phase space with either ME or PS – avoid dead regions.

⇒ ME and PS describe the same final state – remove double counting.

[MANGANO — CATANI, KRAUSS, KUHN, WEBBER — LÖNNBLAD — RICHARDSON]



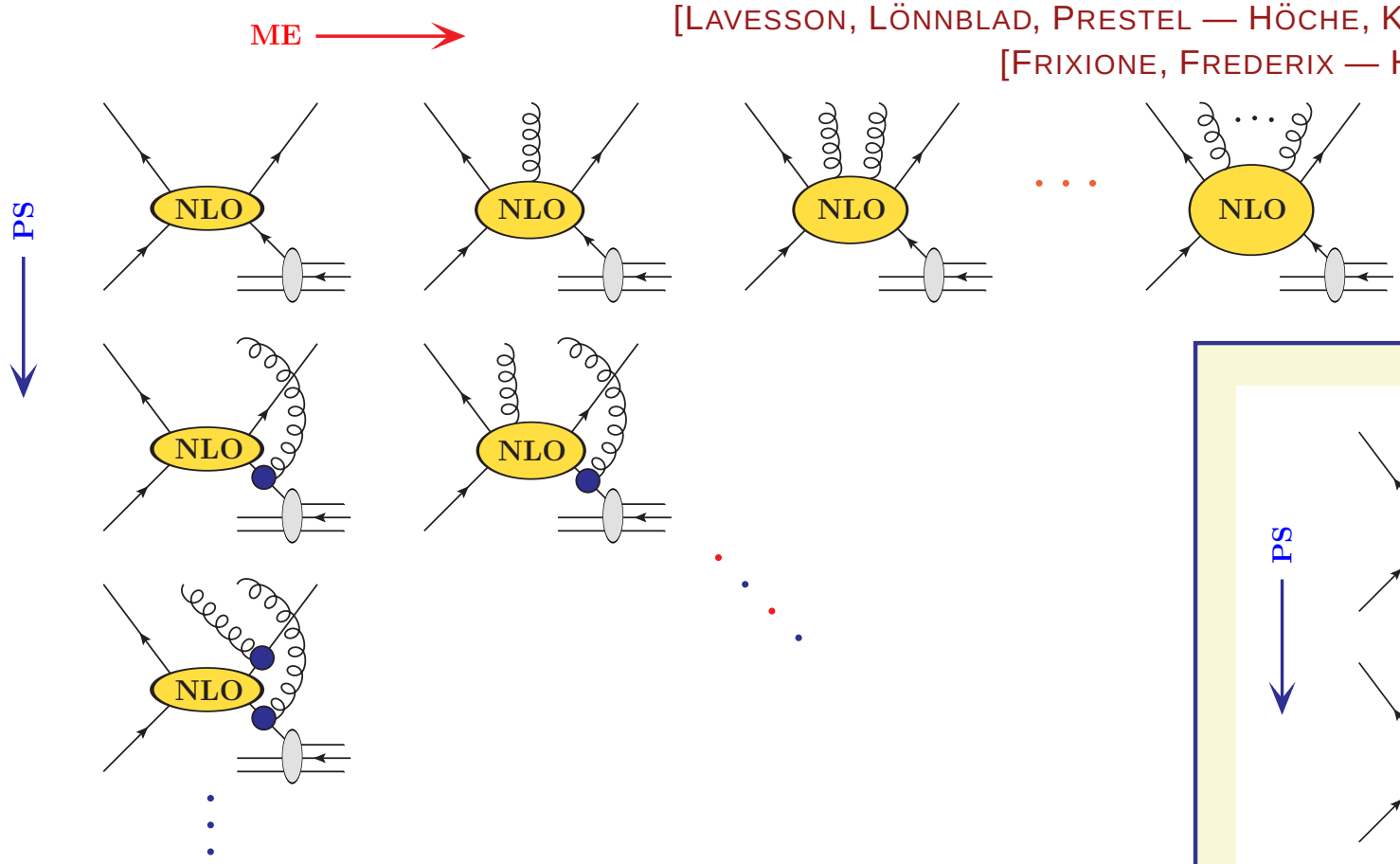
- identical parton multiplicity along diagonal, differently computed however ➡
- separate phase space into "hard" ME and "soft" PS domains, use a (suitable) jet criterion for "hard"/"soft" separation.
- find likely PS history (by "inverted" showering) for n-parton ME to further evolve beyond n partons.

ME+PS ... nowadays necessary tool for "jetty" background simulations.

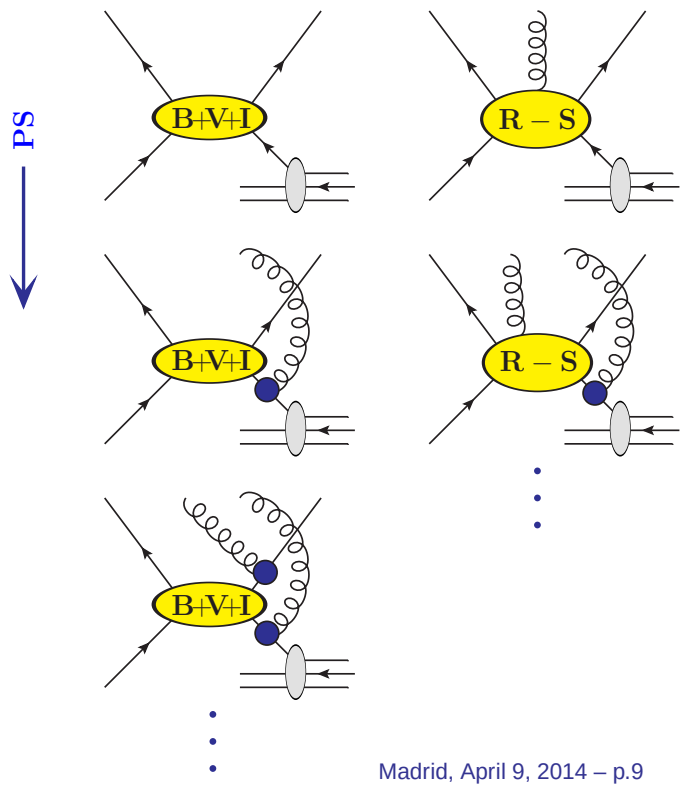
Towards a new standard

ME+PS merging with multiple NLO processes

[Lavesson, Lönnblad, Prestel — Höche, Krauss, Schönherr, Siegert]
[Frixione, Frederix — Hamilton, Nason — Plätzer]

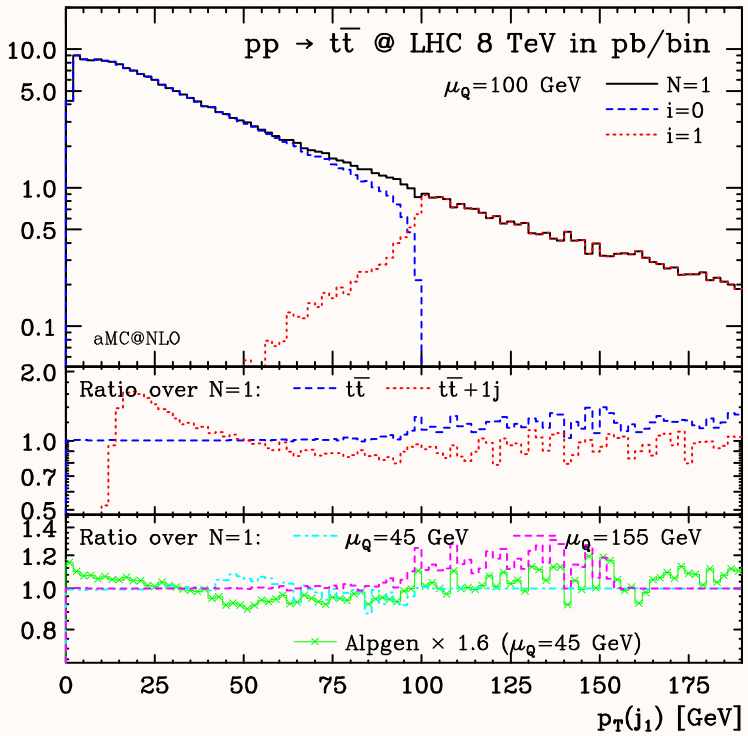


- Per jet bin, NLO+PS matching with extra jet veto.
- Make NLO contributions finite: B+V+I and R-S integrals.
- V from one-loop generators → GoSam, NJet, OpenLoops, etc
  B, R, S, I from → Sherpa;



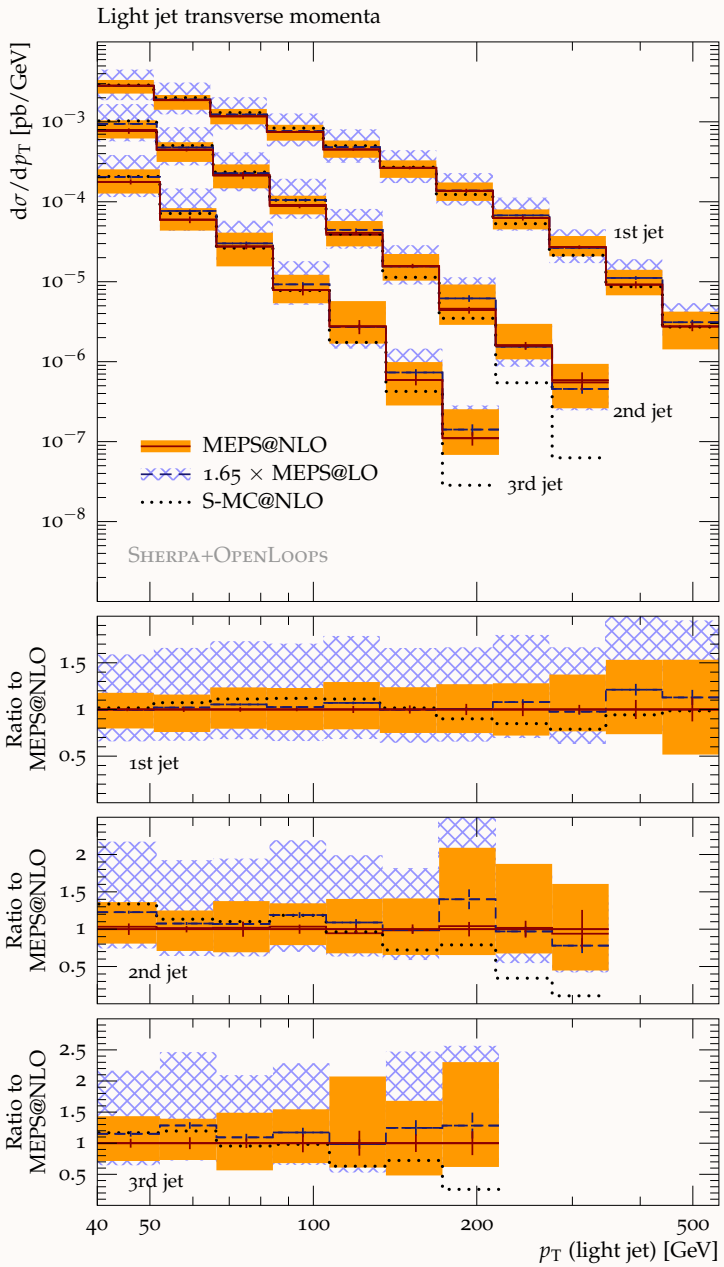
NLO merging in $t\bar{t}$+jets – examples

[Frederix, Frixione, arXiv:1209.6215]



- (upper) FxFx merging for $t\bar{t} + 0, 1$ jet at NLO with aMC@NLO. $\longrightarrow$ small dependence on matching scale
- (right) ME+PS@NLO merging using the Sherpa+OpenLoops framework: top quark pairs with up to 2 jets and LO decays including spin correlation effects. $\longrightarrow$ theory uncertainties reduced to $20 - 30\%$.

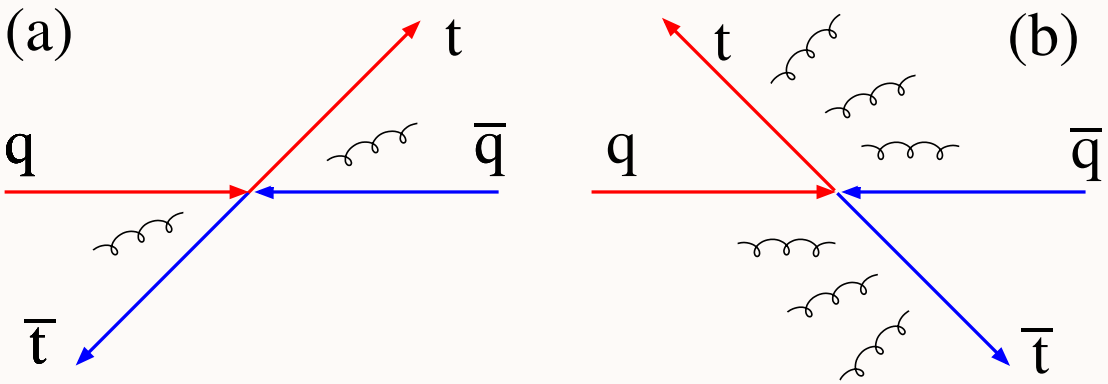
[Höche et al. arXiv:1402.6293]



Quick note on top quark asymmetries

➡ ***Colour coherence in top quark pair production.***

(a) forward (b) backward configurations

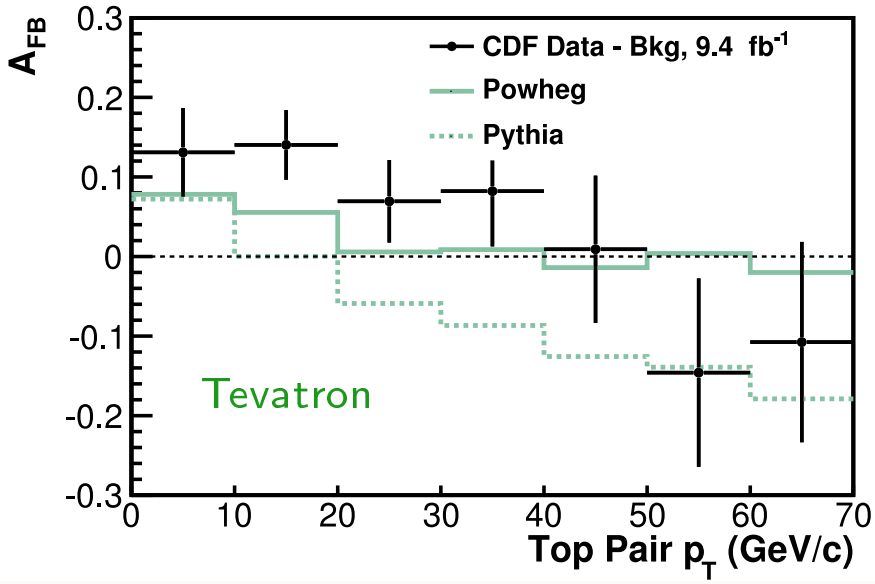


- colour charges more strongly accelerated in "backward" dipoles
- rapidity difference:
  $\Delta y = y_t - y_{\bar{t}}$
  where $y \equiv \frac{1}{2} \ln \frac{E+p_z}{E-p_z}$

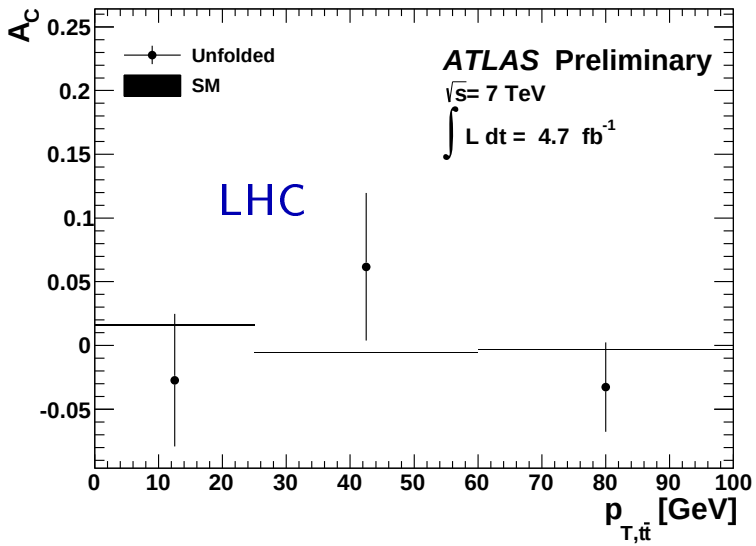
$$A_{\rm FB}(O) = \frac{\left.\frac{d\sigma}{dO}\right|_{\Delta y>0} - \left.\frac{d\sigma}{dO}\right|_{\Delta y<0}}{\left.\frac{d\sigma}{dO}\right|_{\Delta y>0} + \left.\frac{d\sigma}{dO}\right|_{\Delta y<0}}$$

- How accurate are our SM predictions?
  ⇒ Test the new standard in Monte Carlos.

[PLOT BELOW FROM CDF – ARXIV:1211.1003]



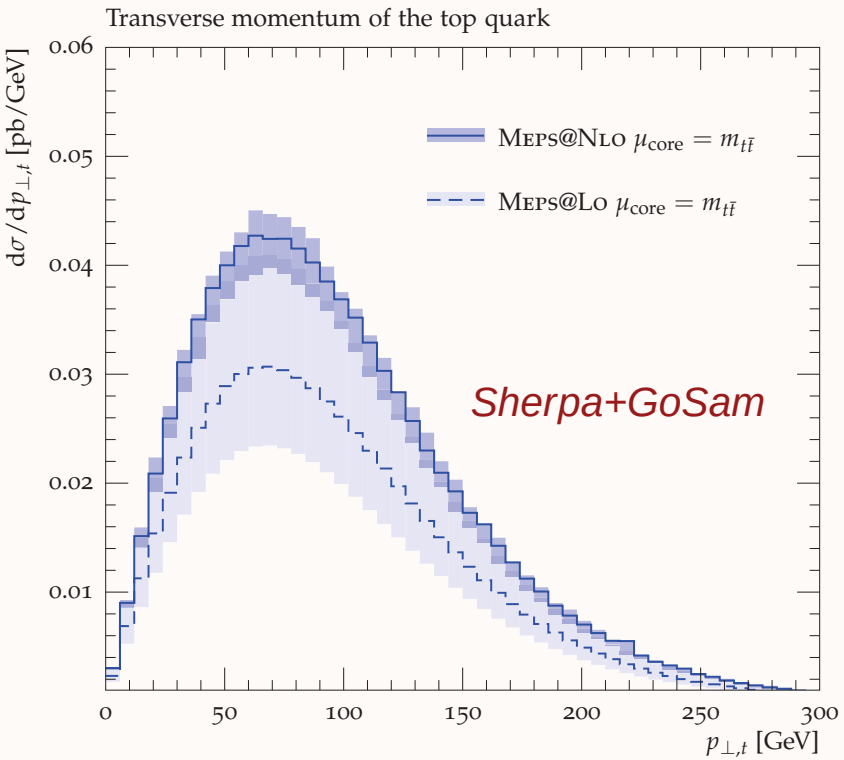
[PLOT BELOW FROM ATLAS-CONF-2013-078]

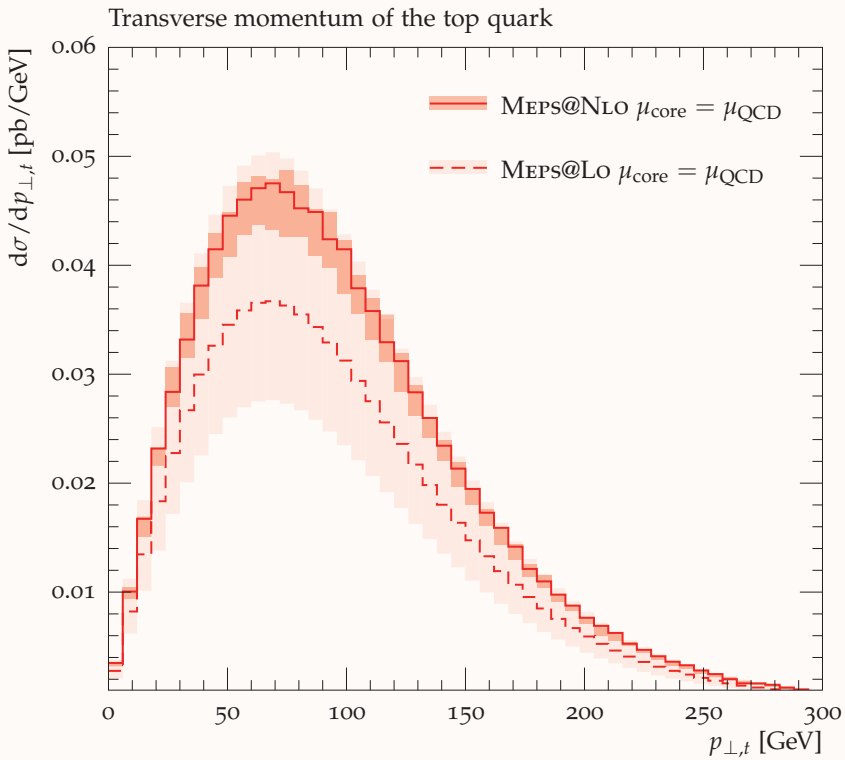


FB differential asymmetry with ME+PS@NLO

[Höche, Huang, Luisoni, Schönherr, Winter, arXiv:1306.2703]

- Scale uncertainties provide us with an estimate of the size of missing higher-order contributions.
- Differential cross sections are more sensitive to conventional scale variations (by factors of 2) than ratios of them, such as A_{FB}. $\Rightarrow$ Different functional forms of the scale definition are needed for a more realistic estimate of the uncertainty.
- We use a scale based on the leading colour flow and compare it to the plain top quark pair mass.





$p\bar{p} \to t\bar{t}$+jets (0,1 @ NLO & virtual MEs from GoSam)

red: $\mu_{\mathrm{core}} = 2|p_i p_j|$

blue: $\mu_{\mathrm{core}} = m_{t\bar{t}}$

perturbative scale (factor) variations &

variation of merging parameter $Q_{\mathrm{cut}} \in \{5, 7, 10\}$ GeV

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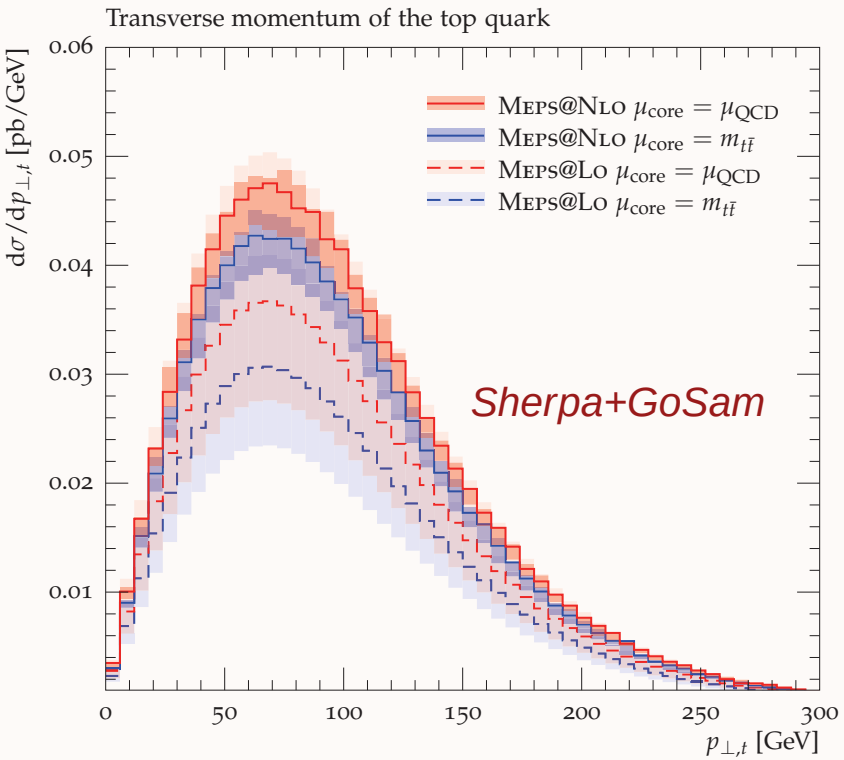

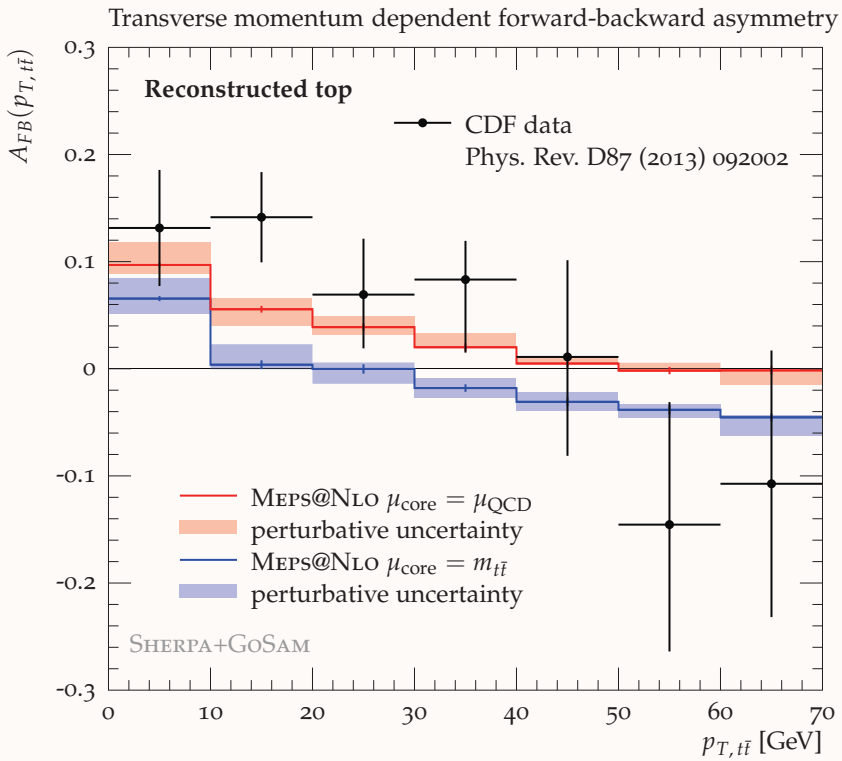

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➡ $A_{\mathrm{FB}}(p_{T,t\bar{t}})$ is QCD NLO accurate in all but the first bin (no EW corrections included).

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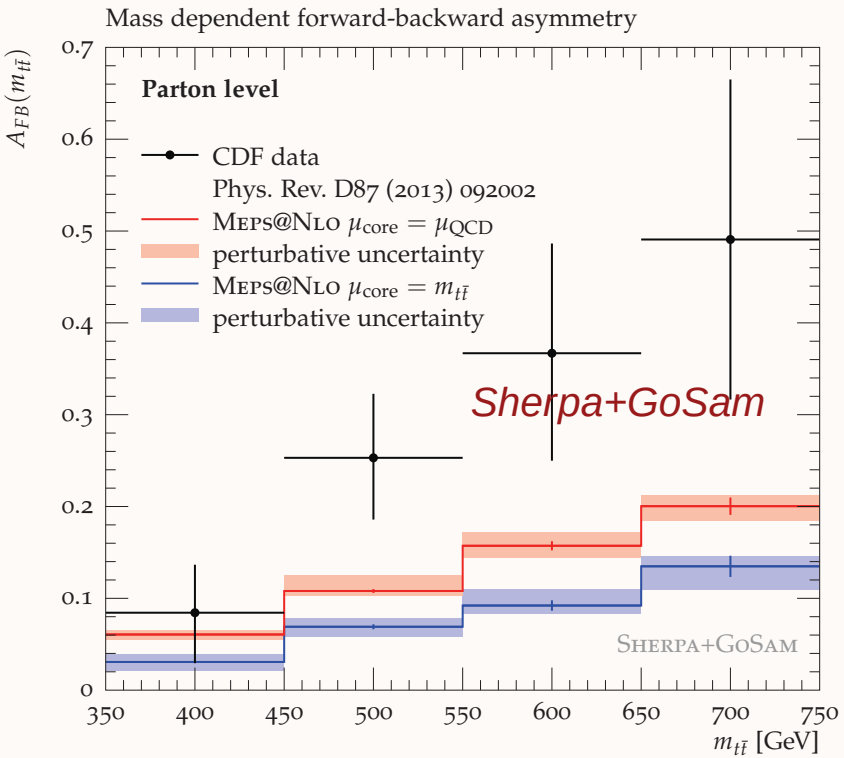

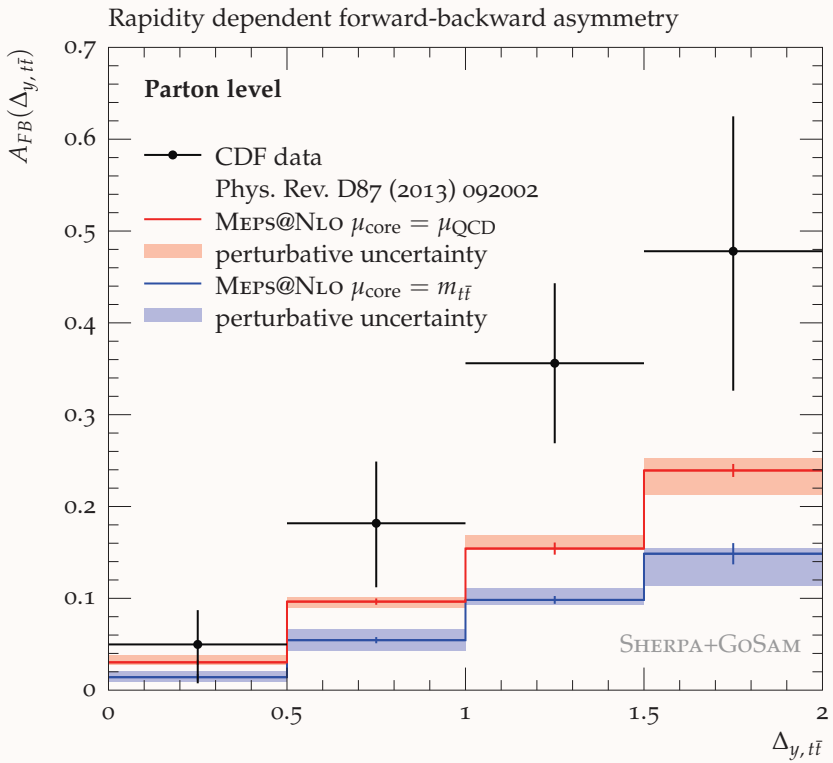

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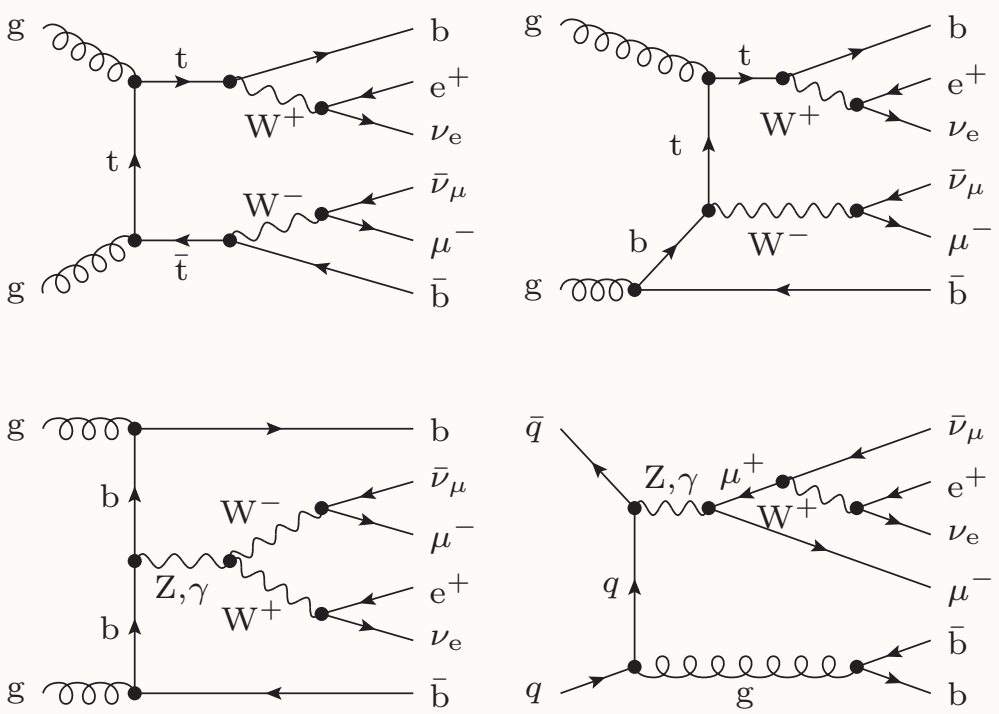
variation of merging parameter $Q_{\mathrm{cut}} \in \{5, 7, 10\}$ GeV

➡ (left) $A_{\mathrm{FB}}(m_{t\bar{t}})$ and (right) $A_{\mathrm{FB}}(|\Delta y|)$: Tevatron situation still remains unclear.

$WWb\bar{b}$ production at NLO

➡ ***New development: bottom quark mass included in calculation.***



- full NLO treatment includes double-, single- and non-resonant contributions
- complex-mass scheme
- finite top-quark and W width effects
- first done in massless b-quark approximation
  [DENNER ET AL. ARXIV:1012.3975, ARXIV:1207.5018]
  [BEVILACQUA ET AL. ARXIV:1012.4230]
- earlier done in NWA where production and decay factorize (neglected contributions are suppressed by powers of $\Gamma_t/m_t \lesssim 1\%$)
  [MELNIKOV, SCHULZE, ARXIV:0907.3090]

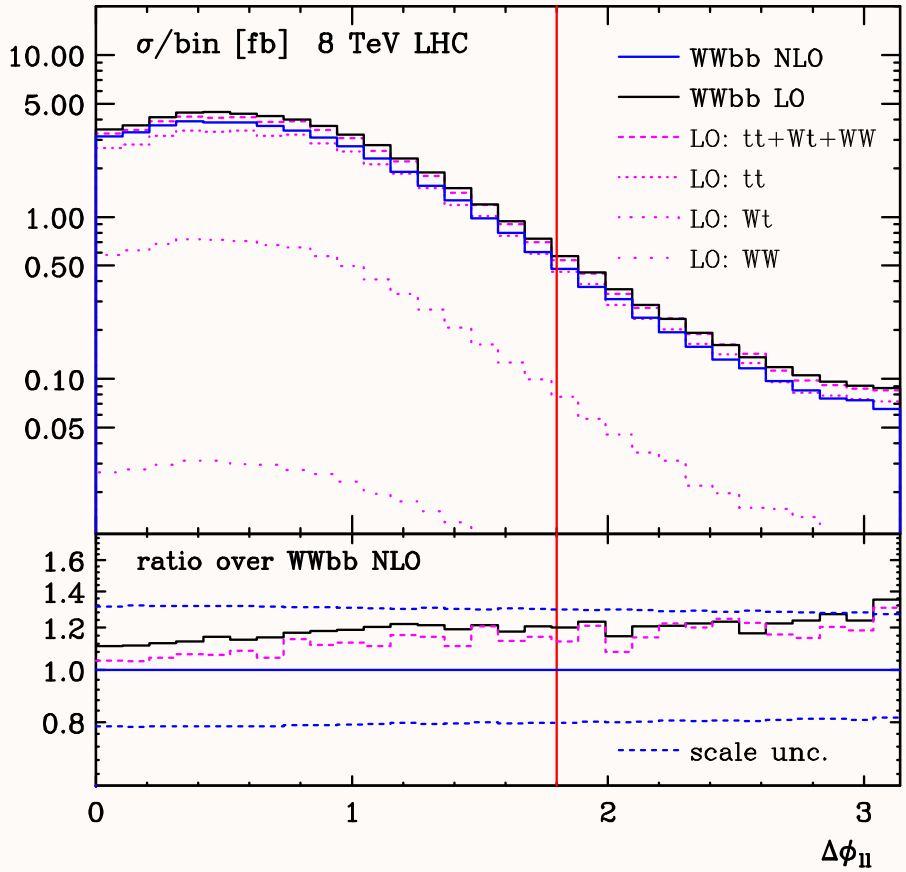
- off-shell and single-top contributions more important in phase-space regions with unresolved b-quarks
- only accessible in calculations with massive b-quarks in the 4-flavour (4F) scheme
- in the 4F, fully differential NLO description of both FS b-jets → permits application of jet vetoes
- → gauge-invariant separation of narrow-top-width contribution and finite-width remainder
- results provided recently by two groups:

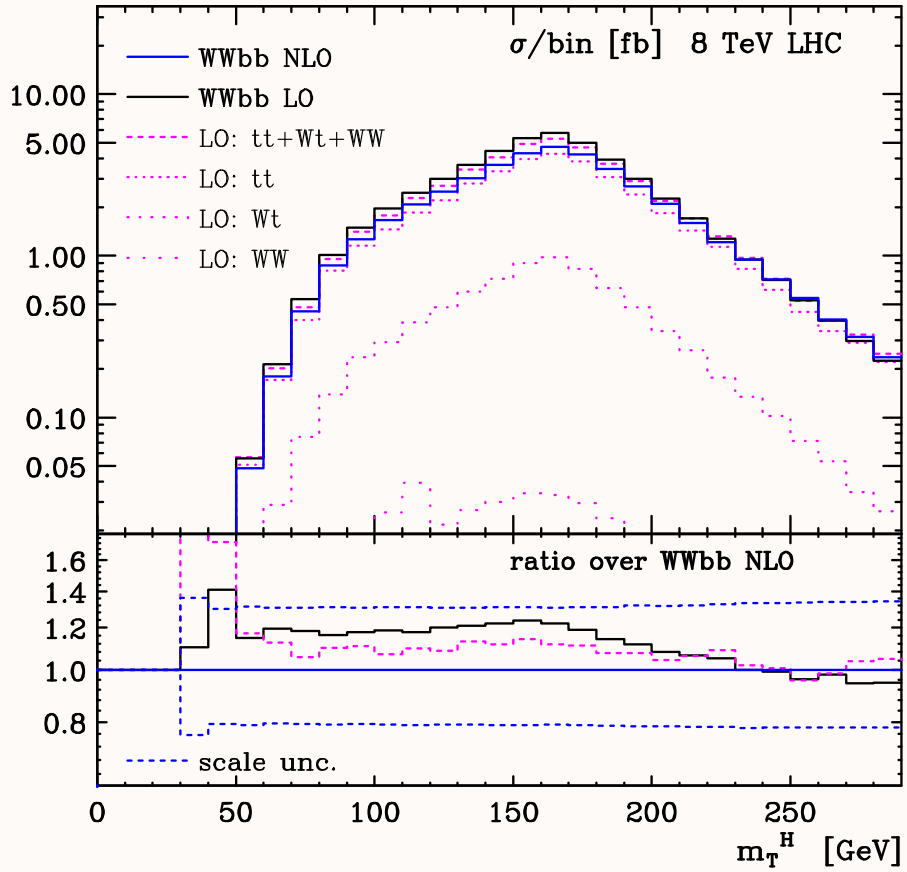
[FREDERIX, ARXIV:1311.4893] [CASCIOLI, KALLWEIT, MAIERHÖFER, POZZORINI, ARXIV:1312.0546]

$WWb\bar{b}$ production at NLO

➡ ***Calculation performed within MadGraph5_aMC@NLO framework.*** [FREDERIX, ARXIV:1311.4893]

- top-quark induced backgrounds in $h \to WW^{(*)} \to ll\nu\nu$ channel at 8 TeV LHC $(\mu_{\mathrm{R,F}} = \hat{H}_T/2)$
- "Higgs measurement" cuts in one-jet bin motivated by ATLAS analysis



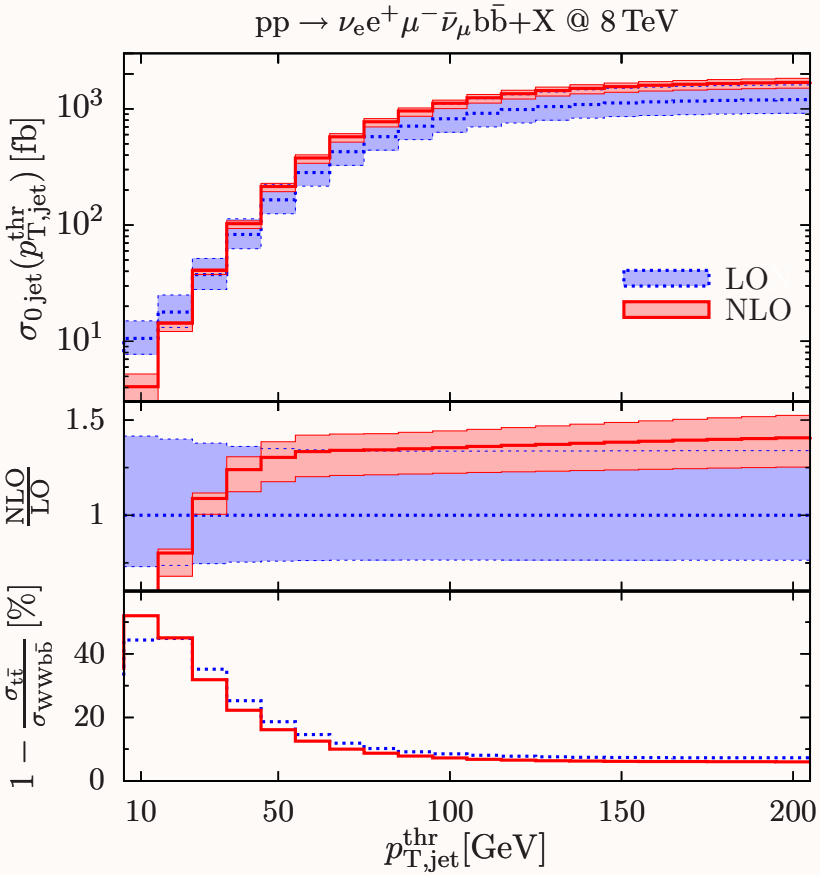


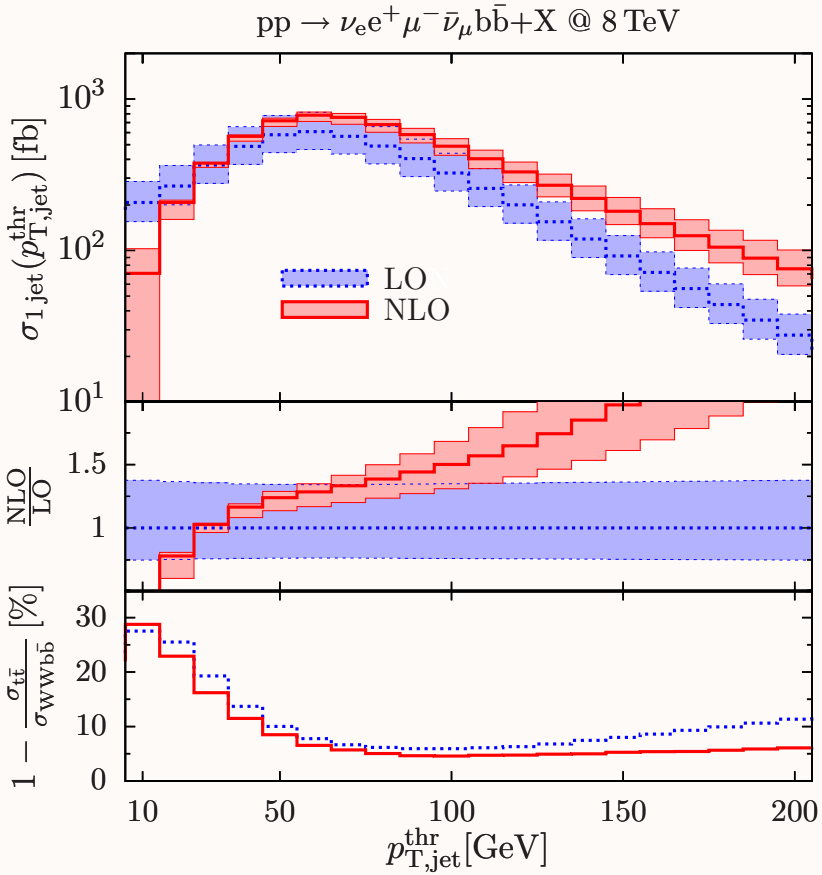
- (left) azimuthal angle separation between leptons, (right) Higgs boson transverse mass
  Higgs boson topology cuts: $m_{ll} < 50$ GeV and $|\Delta\phi_{ll}| < 1.8$

$WWb\bar{b}$ production at NLO

➡ ***OpenLoops + Collier + new in-house NLO MC framework.*** [CASCIOLI ET AL. ARXIV:1312.0546]

- dynamical scale interpolating between $t\bar{t}$ ($\mu^2_{t\bar{t}} = E_{T,t}E_{T,\bar{t}}$) and single-$t$ ($\mu^2_{tW^-} = E_{T,t}E_{T,\bar{b}}$)
- xsec scale uncertainties of $10-15\%$ (similar for $\mu_0 = m_t$), 6% due to finite-t-width corrections





- cross section in exclusive zero- and one-jet bins as a function of jet p_T threshold

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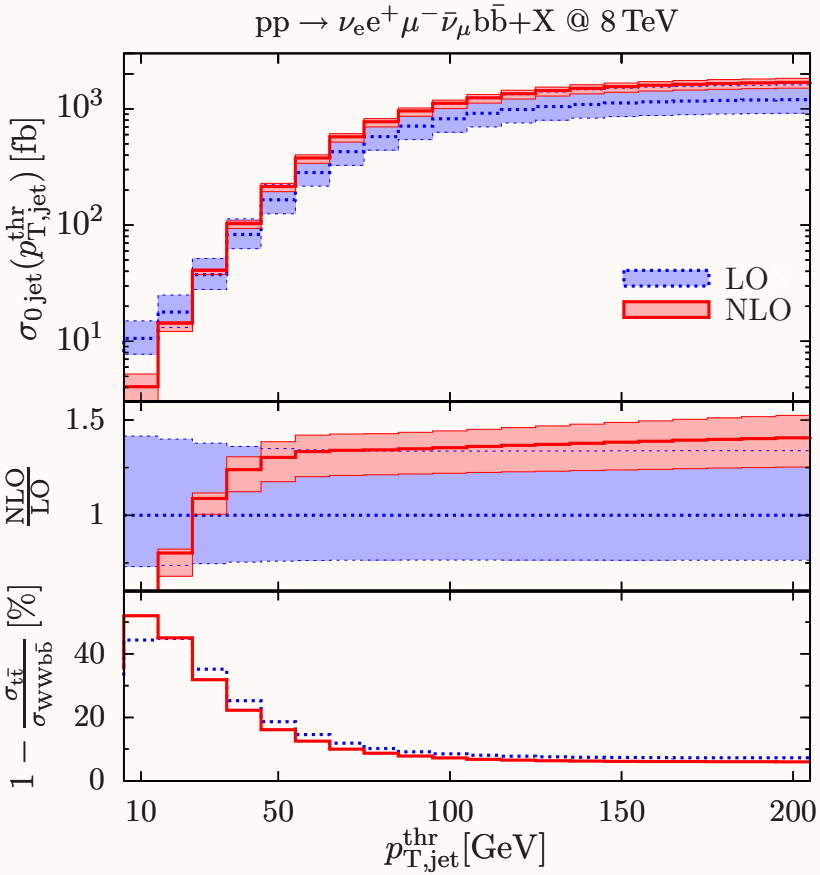
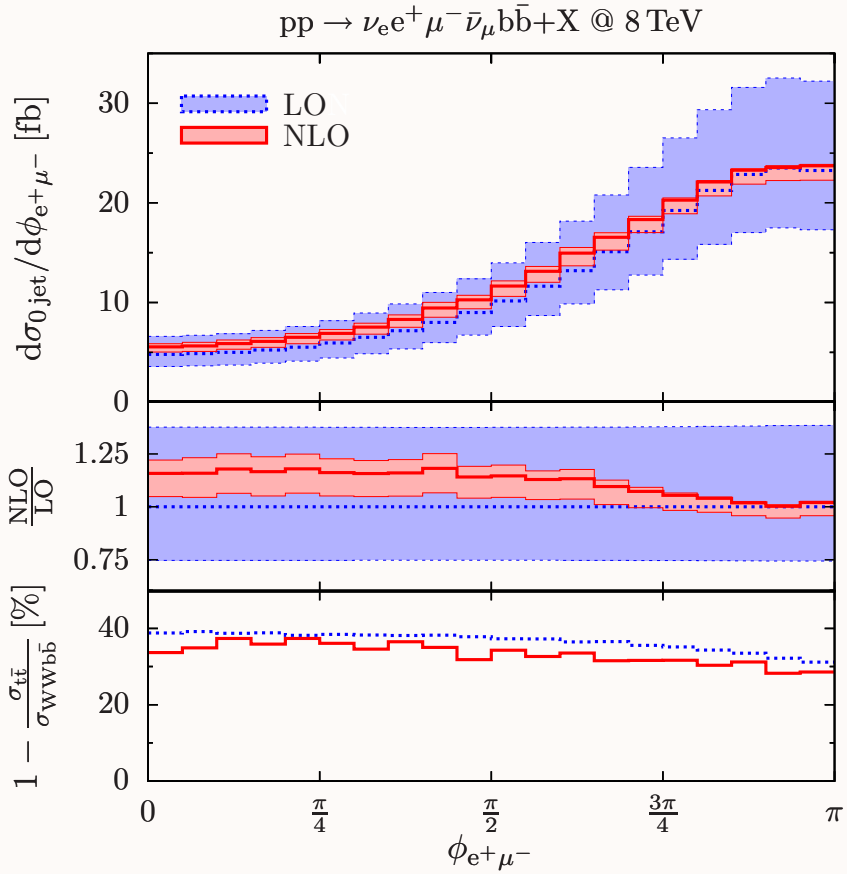




- cross section in exclusive zero- and one-jet bins as a function of jet p_T threshold
- (right) azimuthal angle between leptons (0-jet), finite-t-width effects increase with harsher vetoes

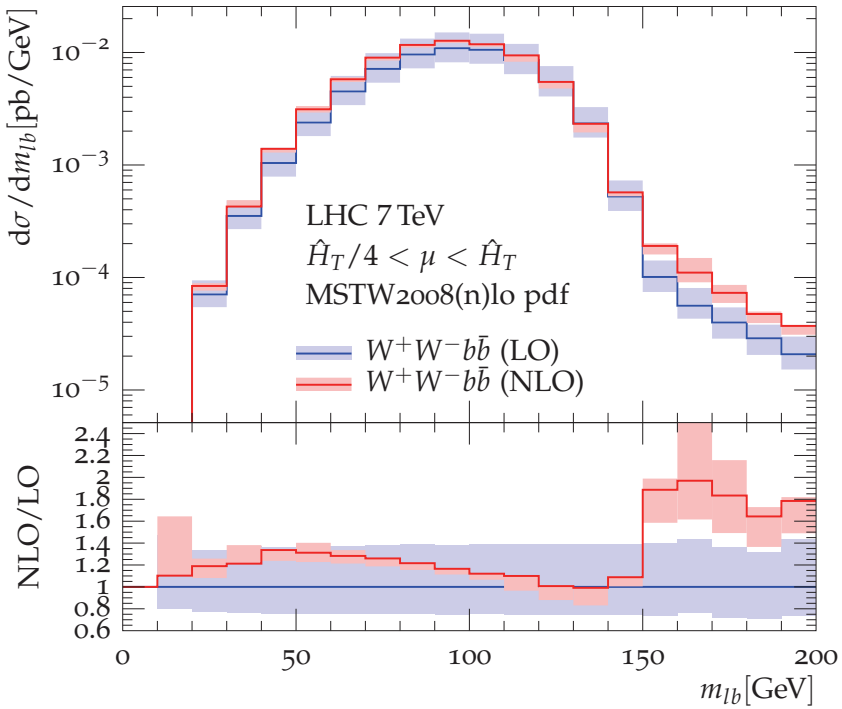
Top quark mass (parameter) determination from

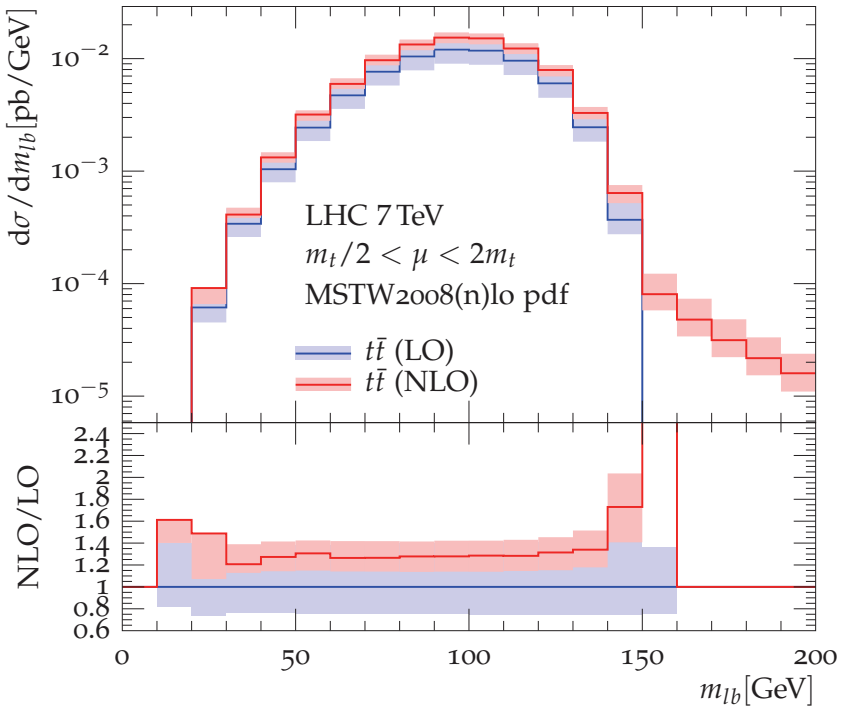
shape of invariant mass distribution of charged lepton and b-jet in WWbb production.

The m_{lb} distribution at NLO

➡ ***Parton-level NLO calculations for $W^+W^-b\bar{b}$ based on GoSam+Sherpa framework.***

(full & factorized calc., 5-flavour scheme, massless b-quarks, two resonant W decaying leptonically @ LO)





- Important NLO corrections to the shape of m_{lb}
- Values of m_{lb} larger than $\sqrt{m_t^2 - m_W^2}$ are kinematically forbidden in narrow width approximation at LO

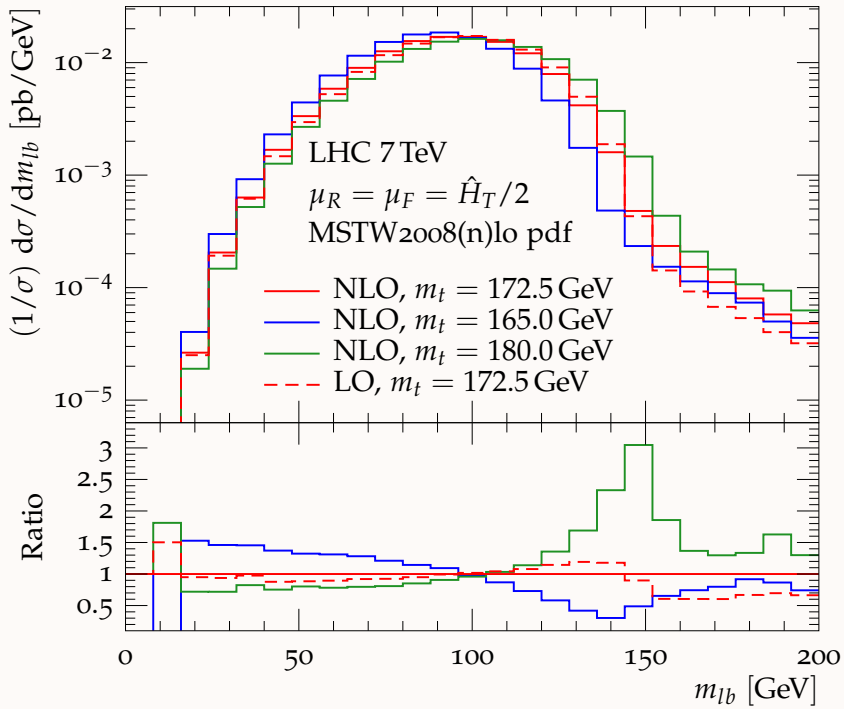
• follow ATLAS strategy: use charged-lepton b-jet pairing minimizing sum of both m_{lb} and average.

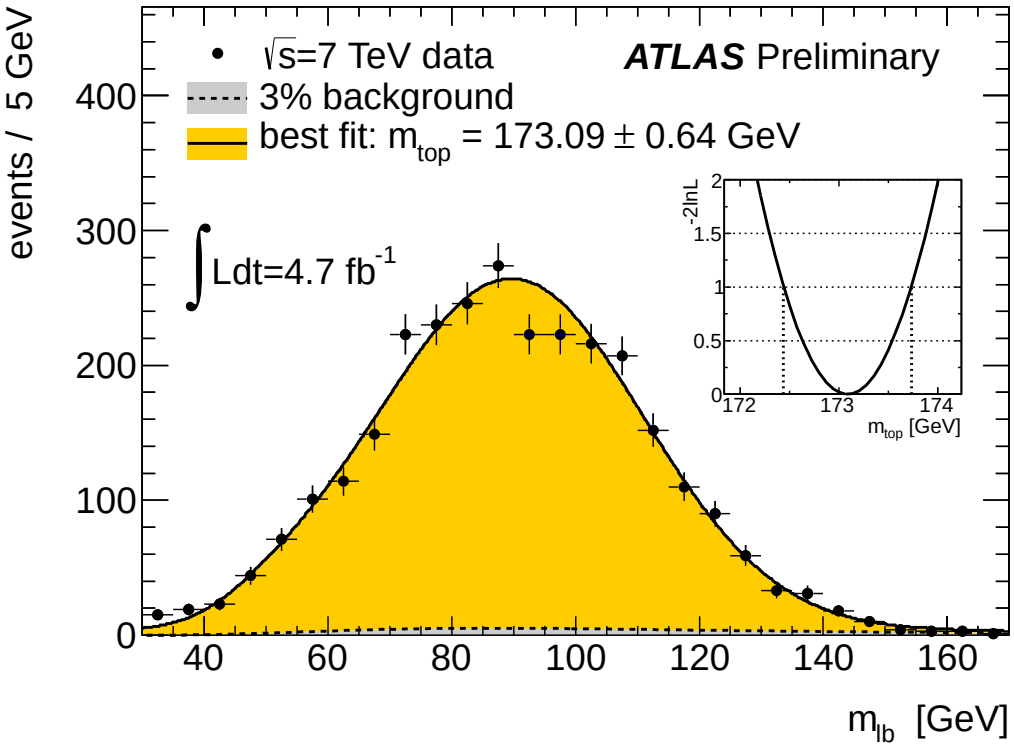
Top quark mass determination using the m_{lb} method

Parametrize "your" theory (m_{lb} predictions).

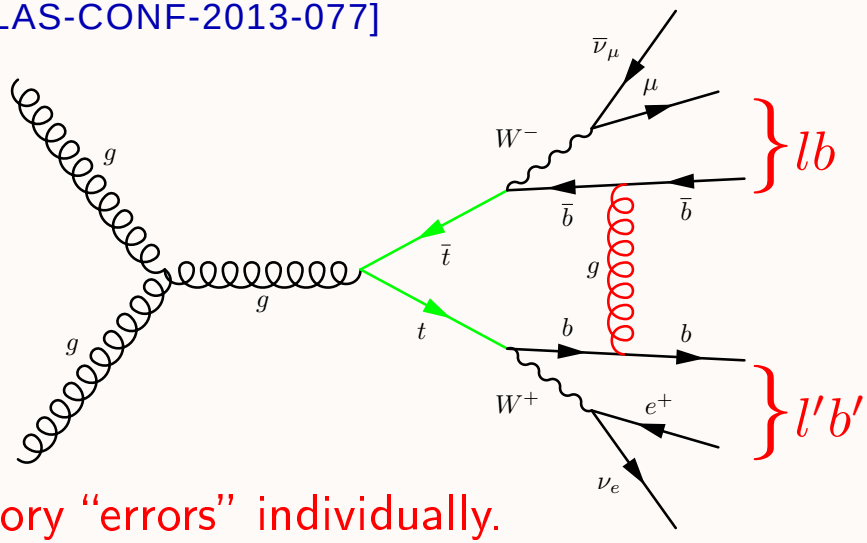
- Full QCD NLO prediction for $W^+W^-b\bar{b}$ in dilepton channel: m_{lb} distribution is sensitive to top quark mass.
- ATLAS uses one-dim. template method to determine m_t. Theory uncertainty has been estimated to 0.8 GeV.

$\rightarrow$ Verify size of th. uncertainties using more advanced calc's!





[ATLAS-CONF-2013-077]



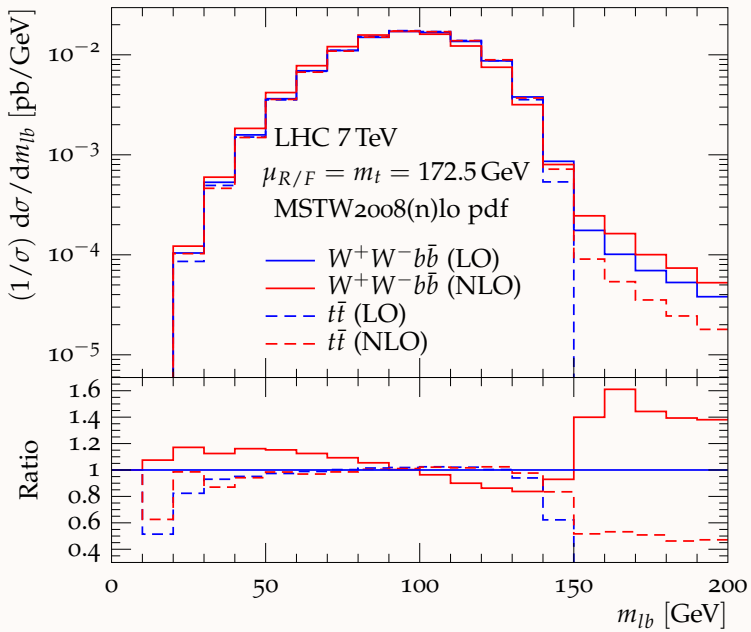
➡ Use pseudo-data to study different types of theory "errors" individually.

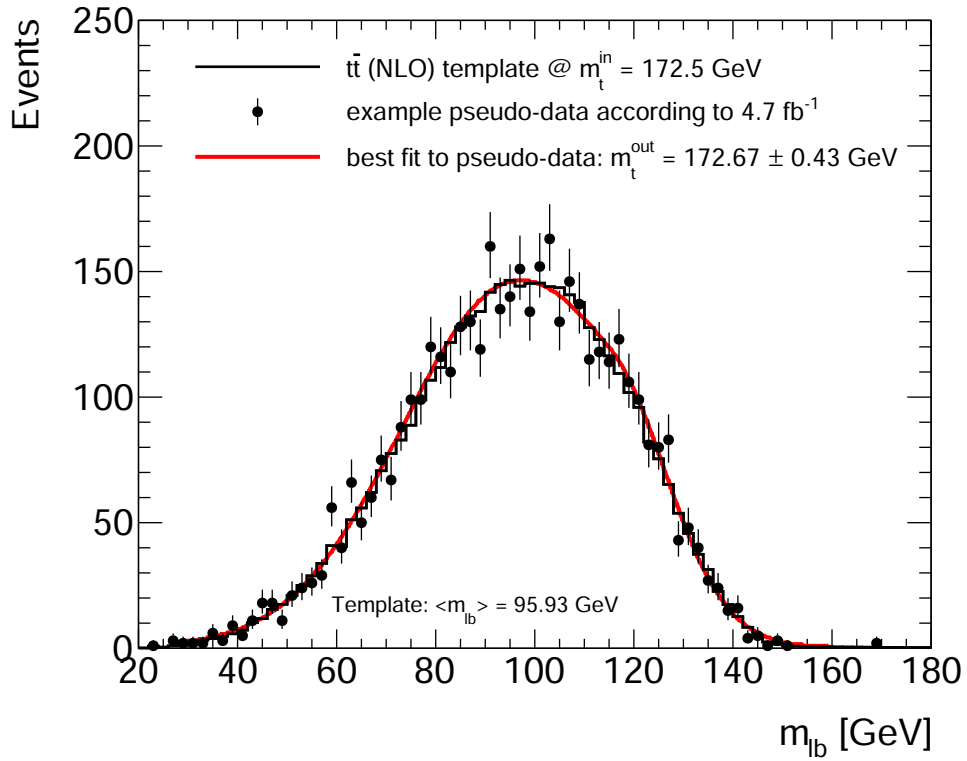
Scale uncertainties and the m_{lb} method

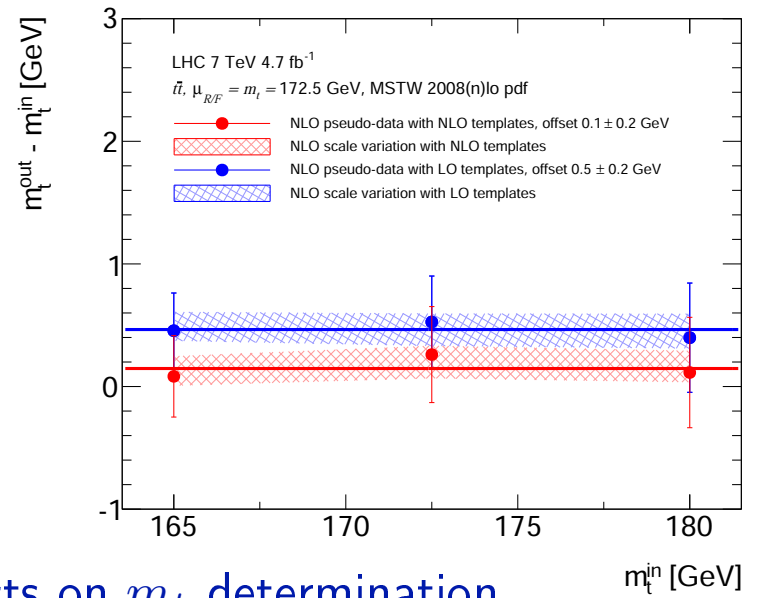
[Heinrich, Maier, Nisius, Schlenk, Winter, arXiv:1312.6659]

Single out effect of NLO scale uncertainties on top mass.

- Use m_{lb} method in a parton-level analysis where we assume that data follows factorized QCD NLO prediction for $t\bar{t}$ with subsequent dilepton decays at LO [pseudo-data].
- Apply/test against the theories given by default scale choice NLO and LO predictions (templates) [hypotheses].







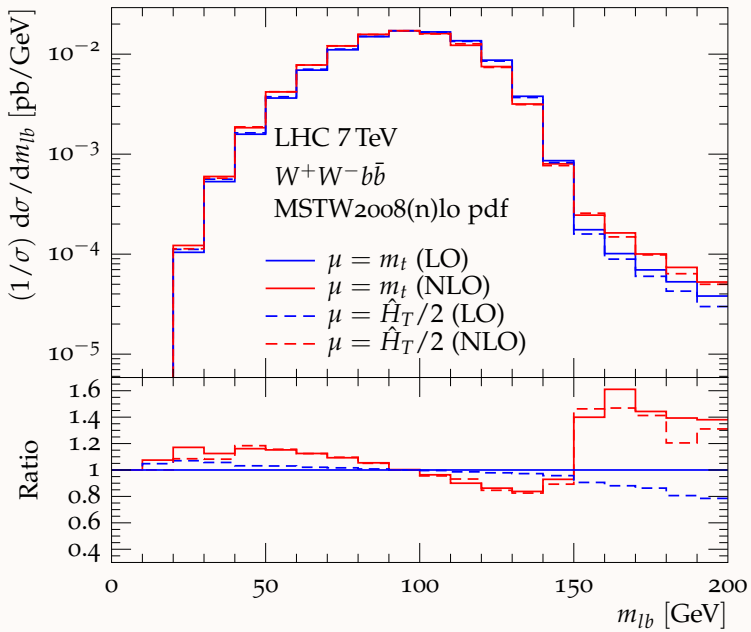
➡ Based on NLO $t\bar{t}$ + LO decays, only small effects on m_t determination.

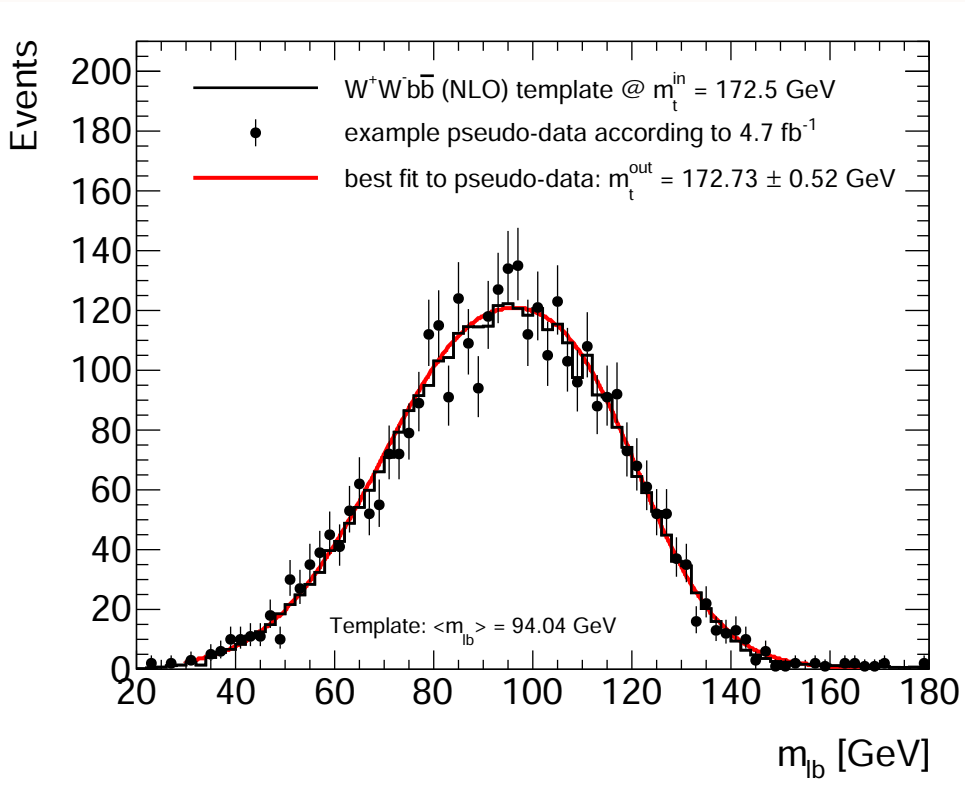
Scale uncertainties and the m_{lb} method

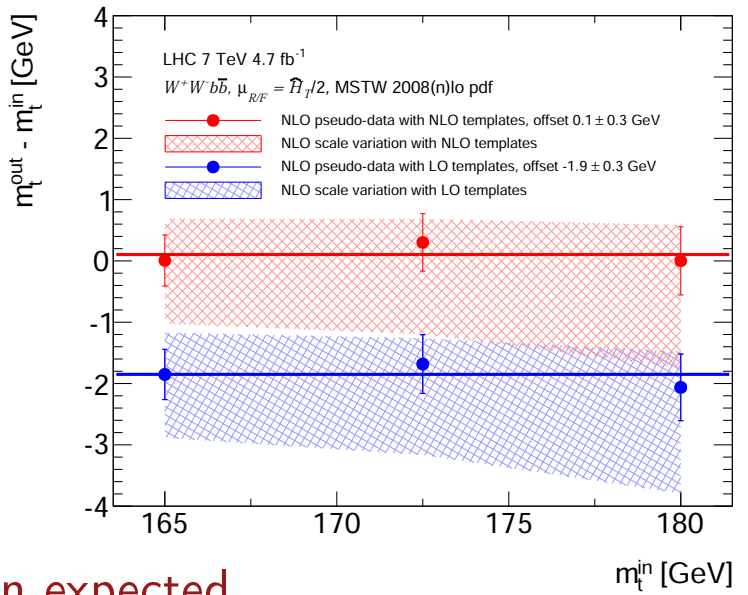
[Heinrich, Maier, Nisius, Schlenk, Winter, arXiv:1312.6659]

Single out effect of NLO scale uncertainties on top mass.

- Use m_{lb} method in a parton-level analysis where we assume that data follows full QCD NLO prediction for dileptonic $W^+W^-b\bar{b}$ [pseudo-data].
- Apply/test against the theories given by default scale choice NLO and LO predictions (templates) [hypotheses].





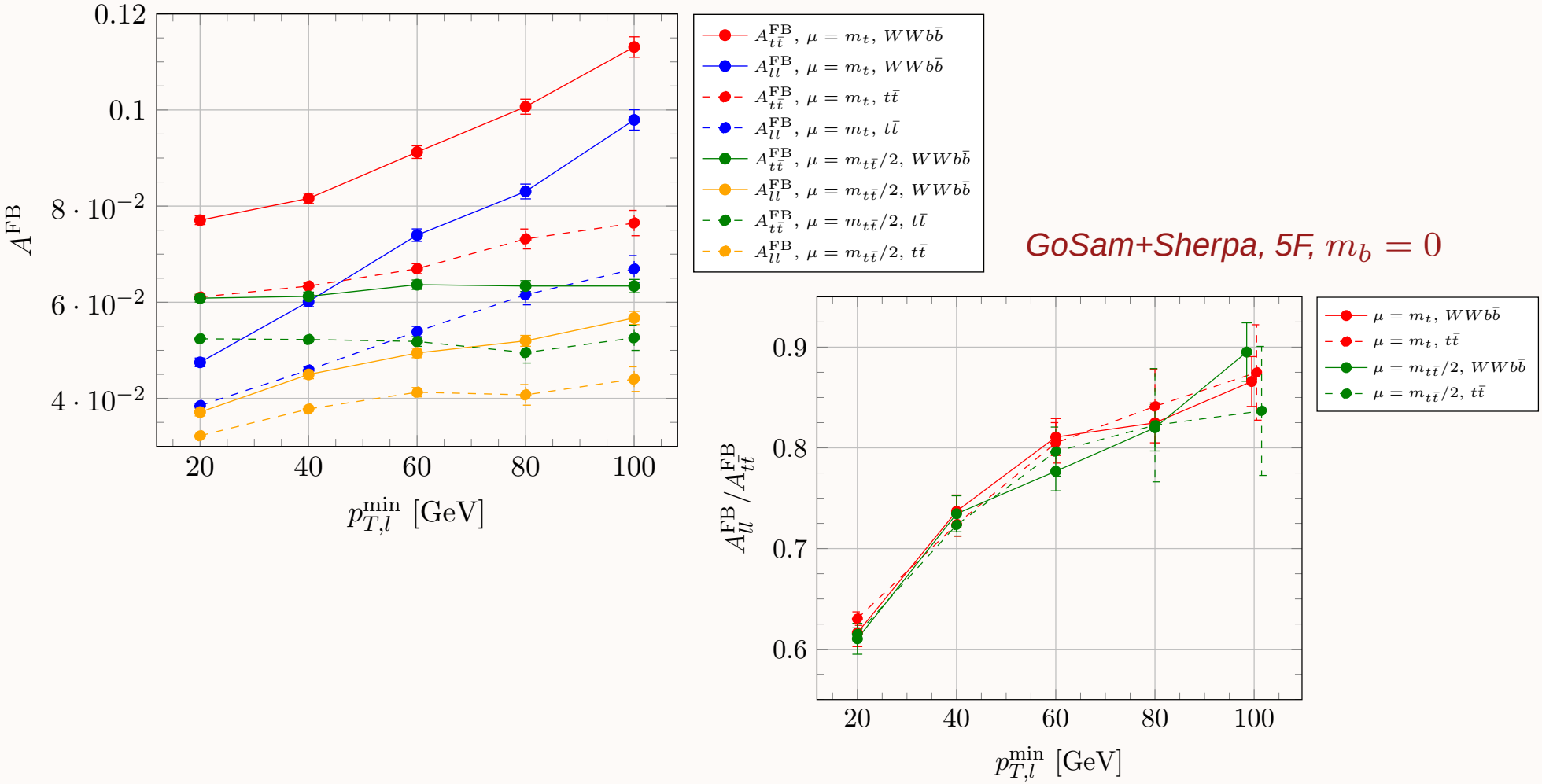


➡ Impacts top quark mass determination more than expected.

Remark: forward–backward asymmetries

[HEINRICH, MAIER, NISIUS, SCHLENK, WINTER, ARXIV:1312.6659]

Compare full vs factorized $WWb\bar{b}$ @ NLO in the context of top quark and lepton-based AFB.



Summary

- Top quark physics has seen great progress over the course of one year (since Freiburg conference), owing to many automated NLO computations.

- Monte Carlos for top physics: standard nowadays is NLO+PS for single top quark, top quark pair and associated production.
  - PowhegBox (and interface to showers). [Nason et al.]
  - MC@NLO and aMC@NLO (and interface to showers). [Frixione et al.]
  - Sherpa with virtual corrections from BlackHat/GoSam/OpenLoops/NJet etc. [Krauss et al.]
  - MatchBox in Herwig++ [Gieseke, Plätzer et al.]
  - UNLOPS in Pythia 8 [Lönnblad, Prestel]
- NLO matrix-element plus parton shower merging produces remarkable results.

- My apologies for being selective. No discussion of
  - single-top production ($\longrightarrow$ S. Frixione's talk)
  - resummed calculations
  - top quark polarization and spin correlations
  - treatment of decays and boosted top quarks
  - theoretical issues regarding top quark mass definition
  - etc.

  in the context of top quark physics.

Summary & Outlook (more specific).

Higher order QCD corrections help narrow the gap between AFB Tevatron measurements and predictions but do not resolve discrepancies completely.

Continuation of pheno studies necessary, in particular for top quark asymmetries at the LHC. Reconstruction and unfolding effects fully understood? Complete NLO predictions for AFB?

Shape uncertainties from scale variations of the full NLO QCD corrections to $WWb\bar{b}$ production result in larger theory errors on the top quark mass determination than expected.

Validation ongoing (NLO in "decay" seems crucial). Parton showering and hadronization effects? Hadron-level predictions wanted.

The end.